STIC Search Report
EIC 1700

STIC Database Tracking Number: 196438

TO: Ben Sackey
Location: REM 5B31
Art Unit : 1626
July 27, 2006

Case Serial Number: 10/751388

From: Kathleen Fuller
Location: EIC 1700
REMSEN 4B28
Phone: 571/272-2505
Kathleen.Fuller@uspto.gov

Search Notes

ACCESS DB # 196438

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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: Ben Sackey Examiner #: 73489 Date: 7/25/06

Art Unit: 1626 Phone Number: 2-0704 Serial Number: 10/751,388

Location (Bldg/Room#):_____ (Mailbox #):_____ Results Format Preferred (circle): PAPER DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Isotopically enriched N-Substituted piperazines & methods for prep

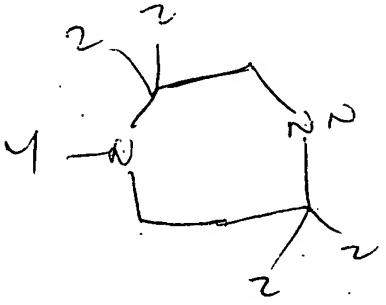
Inventors (please provide full names): Pappin et al.

Earliest Priority Date: 01/05/05

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*



SCIENTIFIC REFERENCE BR
Sci & Tech Inf Ctr
JUL 2 : 2006
Pat. & T.M. Office

Y is a straight or branched C1-6 alky or ether gp.

Z is H, halo, NH2 etc

30

=> FILE REG
FILE 'REGISTRY' ENTERED AT 16:53:26 ON 27 JUL 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 JUL 2006 HIGHEST RN 896142-63-5
DICTIONARY FILE UPDATES: 26 JUL 2006 HIGHEST RN 896142-63-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> FILE HCAPLU
FILE 'HCAPLUS' ENTERED AT 16:53:31 ON 27 JUL 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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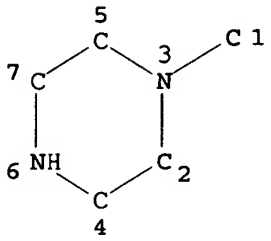
FILE COVERS 1907 - 27 Jul 2006 VOL 145 ISS 5
FILE LAST UPDATED: 26 Jul 2006 (20060726/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D QUE
L16 STR



32,944 structures from query

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE

L21	32944	SEA FILE=REGISTRY SSS FUL L16	
L25	8	SEA FILE=REGISTRY ABB=ON	L21 AND 13C
L26	5	SEA FILE=REGISTRY ABB=ON	L21 AND 14C
L28	3	SEA FILE=REGISTRY ABB=ON	L21 AND 16C
L32	2	SEA FILE=REGISTRY ABB=ON	L21 AND DEUT?
L34	2	SEA FILE=REGISTRY ABB=ON	L21 AND TRITIUM
L35	20	SEA FILE=REGISTRY ABB=ON	(L25 OR L26) OR L28 OR L32 OR L34
L36	19	SEA FILE=HCAPLUS ABB=ON	L35
L37	17	SEA FILE=HCAPLUS ABB=ON	L36(L)PREP/RL
L38	19849	SEA FILE=HCAPLUS ABB=ON	L21
L39	6	SEA FILE=HCAPLUS ABB=ON	L38(L)PREP/RL(L)ISOTOP?
L40	29	SEA FILE=HCAPLUS ABB=ON	L38(L)PREP/RL AND ISOTOP?
L42	40	SEA FILE=HCAPLUS ABB=ON	L37 OR L39 OR L40

labeled

=> D L42 BIB ABS HITIND HITSTR 1-40

L42 ANSWER 1 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1078248 HCAPLUS
DN 143:360127
TI Preparation of diagnostic and therapeutic alkyl piperidine/piperazine compounds for neuron imaging and treating neurodegenerative disease
IN Elmaleh, David R.; Songwoon, Choi; Fishman, Alan J.
PA USA
SO U.S. Pat. Appl. Publ., 21 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005222166	A1	20051006	US 2004-814118	20040331
PRAI	US 2004-814118		20040331		

OS MARPAT 143:360127
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Piperidine or piperazine compds. useful for treating neurodegenerative diseases characterized by the lack of dopamine neurons activity or for imaging the dopamine neurons are provided. The compds. are characterized by the formulas I-V : m = 1-6; X, Y, Z1, Z2, and Z3 = H, halo, haloalkyl, alkyl, aryl, (C1-C6) alkoxy, N-alkyl,(C2-C6) acyloxy, N-alkylene, -SH, -SR, wherein R is from the same group as R1 and R2, NH2, NO, CN, OH, COOR6, C(O)NR5R4, NR3R2, or S(O)kR1 wherein k = 1 or 2 and R1 to R6 = H or (C1-C6)alkyl; R1 and R2 = H, (C1-C6) alkyl, hydroxyalkyl or mercaptoalkyl, -COOR1, CN, (C1-C6)alkenyl, (C2-C6)alkynyl, or (un)substituted 1,2,4-oxadiazol-5-yl; R7= H, O or Ph; R8 = H, Ph, halophenyl, nitrophenyl, pyridyl, piperonyl or sulfoxonitrophenyl; W = O or S; T = NH2 or C1-C6 aminoalkyl; A = N or C; T= C1-C6 alkyl or sulfonyl; Q=NH2 or C1-C6 amino alkyl.

IC ICM A61K031-496
ICS A61K031-495; A61K031-445

INCL 514253010; 544360000; 544386000; 544398000; 546225000; 514255040; 514317000

CC 1-11 (Pharmacology)
Section cross-reference(s): 8, 27, 28

IT 728945-86-6P, 2-Oxo-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate **728945-88-8P**, 2-Phenyl-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate 728945-90-2P, 1-Phenyl-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate 728945-92-4P, 1-(2-Fluorophenyl)-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate 728945-94-6P, 1-(4-Fluorophenyl)-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate 728945-96-8P, 1-(2-Chlorophenyl)-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate 728945-98-0P, 1-(3-Chlorophenyl)-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate 728946-00-7P, 1-(4-Chlorophenyl)-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate 728946-02-9P, 1-(2-Methoxyphenyl)-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate 728946-04-1P, 1-[3-(Trifluoromethyl)phenyl]-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate 728946-06-3P, 1-[4-[4-[4-[Bis(4-fluorophenyl)methoxy]butyl]piperazin-1-yl]phenyl]ethanone oxalate 728946-08-5P, 1-(4-Nitrophenyl)-4-[1-[bis(4-fluorophenyl)methoxy]butan-4-yl]piperazine oxalate 728946-10-9P, 1-[4-[Bis(4-fluorophenyl)methoxy]butyl]-4-(pyridin-2-yl)piperazine oxalate 728946-12-1P, 1-Benzoyl-4-[1-[bis(4-fluorophenyl)methoxy]butan-4-yl]piperazine oxalate 728946-14-3P, 1-[(Benzodioxol-5-yl)methyl]-4-[4-[bis(4-fluorophenyl)methoxy]butyl]piperazine oxalate 728946-16-5P, 1-[4-[Bis(4-fluorophenyl)methoxy]butyl]-4-(4-nitrophenylsulfonyl)piperazine oxalate 866006-22-6P 866006-23-7P 866006-24-8P 866006-25-9P 866006-26-0P 866006-28-2P 866006-29-3P 866006-30-6P 866006-31-7P 866006-32-8P 866006-33-9P 866006-36-2P 866006-37-3P 866006-38-4P 866006-39-5P
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(drug candidate; preparation of diagnostic and therapeutic alkyl piperidine/piperazine compds. for neuron imaging and treating neurodegenerative disease)

IT 173186-93-1P, 1-[Bis(4-fluorophenyl)methoxy]-4-chlorobutane **728945-84-4P**, 1-[4-[Bis(4-fluorophenyl)methoxy]butyl]piperazine dioxalate
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(drug candidate; preparation of diagnostic and therapeutic alkyl

piperidine/piperazine compds. for neuron imaging and treating neurodegenerative disease)

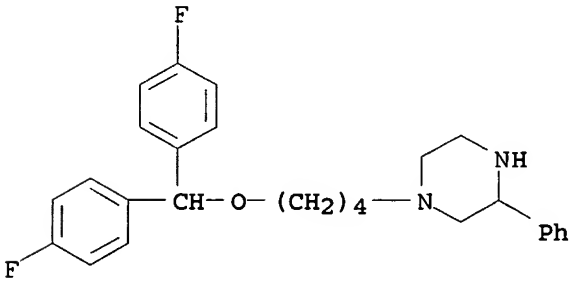
IT 7553-56-2D, Iodine, **isotopes**, complexes with bisarylmethoxybutyl piperazines, biological studies 378784-45-3D, Technetium-99m, complexes with bisarylmethoxybutyl piperazines, biological studies 866006-41-9D, complexes with technetium-99m or iodine **isotopes**
RL: DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
(preparation of diagnostic and therapeutic alkyl piperidine/piperazine compds. for neuron imaging and treating neurodegenerative disease)

IT **728945-88-8P**, 2-Phenyl-4-[4-[bis(4-fluorophenyl)methoxy]butyl]pipe razine oxalate
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(drug candidate; preparation of diagnostic and therapeutic alkyl piperidine/piperazine compds. for neuron imaging and treating neurodegenerative disease)

RN 728945-88-8 HCAPLUS
CN Piperazine, 1-[4-[bis(4-fluorophenyl)methoxy]butyl]-3-phenyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

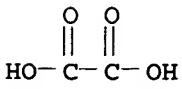
CM 1

CRN 728945-87-7
CMF C27 H30 F2 N2 O



CM 2

CRN 144-62-7
CMF C2 H2 O4



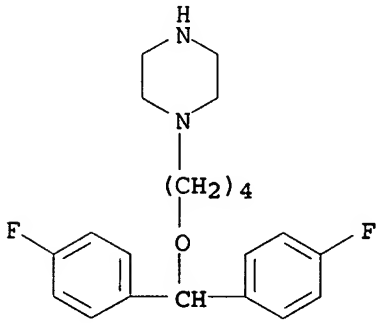
IT **728945-84-4P**, 1-[4-[Bis(4-fluorophenyl)methoxy]butyl]piperazine dioxalate
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(drug candidate; preparation of diagnostic and therapeutic alkyl piperidine/piperazine compds. for neuron imaging and treating neurodegenerative disease)

RN 728945-84-4 HCAPLUS
CN Piperazine, 1-[4-[bis(4-fluorophenyl)methoxy]butyl]-, ethanedioate (1:2)

(9CI) (CA INDEX NAME)

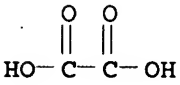
CM 1

CRN 728945-83-3
CMF C21 H26 F2 N2 O



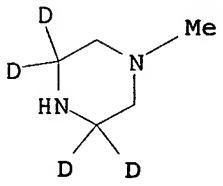
CM 2

CRN 144-62-7
CMF C2 H2 O4



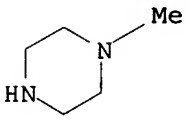
L42 ANSWER 2 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:619662 HCAPLUS
DN 144:254085
TI Syntheses of [14C] and [2H4]PD0205520, an inhibitor of the tyrosine kinase activity of the epidermal growth factor receptor
AU Zhang, Yinsheng; Huang, Yun; Huang, Che C.
CS Radiochemistry Group, Chemical R&D, Michigan Pharmaceutical Sciences, Pfizer Inc., Kalamazoo, MI, 49007, USA
SO Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(7), 485-496
CODEN: JLCRD4; ISSN: 0362-4803
PB John Wiley & Sons Ltd.
DT Journal
LA English
AB 5-(4-Methyl-piperazin-1-yl)pent-2-ynoic acid {4-[(3-chloro-4-fluoro-phenyl)amino]pyrido[3,4-d]pyrimidin-6-yl}amide, PD0205520, was under investigation as a potential inhibitor of the tyrosine kinase (TK) activity of the epidermal growth factor receptor (EGFR) for cancer treatment. Both radio- and stable-**isotope**-labeled compds. were required for drug absorption, distribution, metabolism and excretion (ADME) and quant. mass spectrometry bio-anal. studies. PD0205520 14C-labeled in the pyrimidine ring system was prepared in seven steps in an overall radiochem. yield of 26% from [14C]thiourea. PD0205520 2H-labeled in the piperazine ring was synthesized in four steps in a 32% overall yield.
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

IT **Isotope** indicators
(preparation of carbon-14- and deuterium-labeled PD0205520)
IT 6277-35-6P 60725-35-1P 88234-15-5P 171178-41-9P 171178-42-0P
171178-43-1P 212632-10-5P 877154-60-4P 877154-61-5P 877154-62-6P
877154-63-7P 877154-64-8P **877154-67-1P** 877154-68-2P
877154-69-3P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of carbon-14- and deuterium-labeled PD0205520)
IT 877154-65-9P **877154-66-0P** 877154-70-6P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of carbon-14- and deuterium-labeled PD0205520)
IT **877154-67-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of carbon-14- and deuterium-labeled PD0205520)
RN 877154-67-1 HCAPLUS
CN Hydrochloric acid-d, compd. with 4-methylpiperazine-2,2,6,6-d4 (2:1) (9CI) (CA INDEX NAME)



●2 DCl

IT **877154-66-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of carbon-14- and deuterium-labeled PD0205520)
RN 877154-66-0 HCAPLUS
CN Piperazine, 1-methyl-, labeled with deuterium (9CI) (CA INDEX NAME)



RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 3 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:592130 HCAPLUS
DN 143:115574
TI Preparation of **isotopically** enriched N-substituted piperazines
IN Pappin, Darryl J. C.; Pillai, Sasi; Coull, James M.
PA Applera Corp., USA
SO U.S. Pat. Appl. Publ., 29 pp.
CODEN: USXXCO
DT Patent
LA English

FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005148773	A1	20050707	US 2004-751388	20040105
	WO 2005068446	A1	20050728	WO 2005-US223	20050105

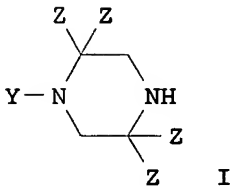
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI	US 2004-751353	A	20040105
	US 2004-751354	A	20040105
	US 2004-751387	A	20040105
	US 2004-751388	A	20040105
	US 2004-822639	A	20040412
	US 2004-852730	A	20040524

OS MARPAT 143:115574

GI



I

AB **Isotopically** enriched N-substituted piperazines (I) or salts thereof, comprising one or more heavy atom **isotopes** (Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or fluorine atoms; Z = independently H, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H or F atoms, a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms), or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group; wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms; wherein the N-methylpiperazine is **isotopically** enriched with either of 13C and/or 15N) are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino

acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like (no data). Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

IC ICM C07D241-04

INCL 544358000

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 6, 80

ST **isotopically** enriched methylpiperazine prepn isobaric labeling reagent; methylpiperazineacetic acid **isotope** labeled prepn isobaric labeling reagent

IT **Isotope** indicators
(preparation of **isotopically** enriched N-substituted piperazines as isobaric labeling reagents)

IT **Isotopomers**
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(preparation of **isotopically** enriched N-substituted piperazines as isobaric labeling reagents)

IT 856188-20-0P
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of **isotopically** enriched N-substituted piperazines as isobaric labeling reagents)

IT 79-08-3, Bromoacetic acid 87-86-5, Pentachlorophenol 109-01-3, N-Methylpiperazine 407-25-0, Trifluoroacetic anhydride 554-84-7, 3-Nitrophenol 658-78-6, Trifluoroacetic acid p-nitrophenyl ester 920-66-1, 1,1,1,3,3,3-Hexafluoropropan-2-ol 1737-40-2, Trifluoroacetic acid 3-nitrophenyl ester 4530-20-5 5625-52-5 6066-82-6, N-Hydroxysuccinimide 13200-60-7, Sarcosine ethyl ester 14314-42-2, Water-18O 14533-84-7, Trifluoroacetic acid pentafluorophenyl ester 18156-74-6, 1-Trimethylsilylimidazole 28230-32-2 52928-63-9, N-Hydroxy-2-pyrrolidinone 53788-49-1 56522-24-8, tert-Butyldimethylsilyl cyanide 61898-49-5 85539-84-0 145590-97-2 856187-95-6, 4-Methylpiperazine-1-acetic acid phenyl ester 857291-01-1 861230-66-2 861230-70-8 861230-78-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of **isotopically** enriched N-substituted piperazines as isobaric labeling reagents)

IT 5672-86-6P, Trifluoroacetic acid pentachlorophenyl ester 5672-89-9P, Trifluoroacetic acid succinimidyl ester 54699-92-2P, 4-Methylpiperazine-1-acetic acid 106665-75-2P 145142-98-9P 145143-00-6P **856187-57-0P** 856187-64-9P 856187-68-3P 856187-72-9P 856187-80-9P 856187-83-2P 856187-92-3P 856188-16-4P 856188-23-3P 856188-27-7P 856188-32-4P **856188-37-9P** **856188-43-7P** **856188-49-3P** 856188-80-2P 856188-88-0P, Trifluoroacetic acid 2-oxopyrrolidin-1-yl ester 856290-54-5P 857027-04-4P 857027-05-5P 857502-96-6P 857502-97-7P 857502-98-8P **857502-99-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of **isotopically** enriched N-substituted piperazines as isobaric labeling reagents)

IT 856187-76-3P 856187-87-6P 856188-02-8P, 4-Methylpiperazine-1-acetic acid 1,1,1,3,3,3-hexafluoropropan-2-yl ester 856188-06-2P

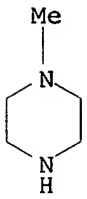
856188-38-0P 856188-44-8P 856188-50-6P
856188-62-0P 857027-09-9P 857027-10-2P 857503-00-5P 857503-01-6P
857503-02-7P 857503-03-8P **857503-04-9P 857503-05-0P**
857503-06-1P 857503-07-2P 857503-08-3P
857503-09-4P 857503-10-7P 857503-11-8P
857503-12-9P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of **isotopically** enriched N-substituted piperazines as isobaric labeling reagents)

IT **856187-57-0P 856188-37-9P 856188-43-7P**
856188-49-3P 857502-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of **isotopically** enriched N-substituted piperazines as isobaric labeling reagents)

RN 856187-57-0 HCAPLUS
CN Piperazine, 1-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

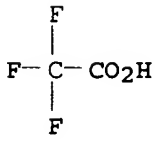
CM 1

CRN 109-01-3
CMF C5 H12 N2

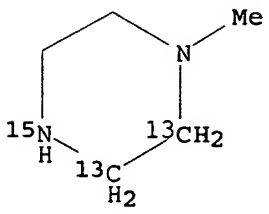


CM 2

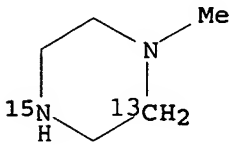
CRN 76-05-1
CMF C2 H F3 O2



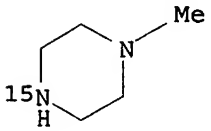
RN 856188-37-9 HCAPLUS
CN Piperazine-2,3-13C2-1-15N, 4-methyl- (9CI) (CA INDEX NAME)



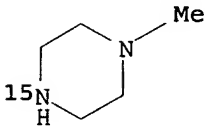
RN 856188-43-7 HCAPLUS
CN Piperazine-3-13C-1-15N, 4-methyl- (9CI) (CA INDEX NAME)



RN 856188-49-3 HCAPLUS
CN Piperazine-15N, 4-methyl- (9CI) (CA INDEX NAME)



RN 857502-99-9 HCAPLUS
CN Piperazine-15N, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

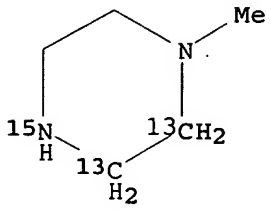


●2 HCl

IT **856188-38-0P 856188-44-8P 856188-50-6P**
857503-04-9P 857503-05-0P 857503-06-1P
857503-07-2P 857503-08-3P 857503-09-4P
857503-10-7P 857503-11-8P 857503-12-9P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of **isotopically** enriched N-substituted piperazines as isobaric labeling reagents)
RN 856188-38-0 HCAPLUS
CN Piperazine-2,3-13C2-1-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

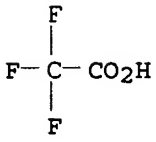
CM 1

CRN 856188-37-9
CMF C5 H12 N2



CM 2

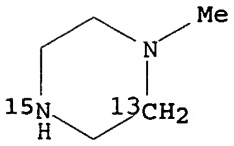
CRN 76-05-1
CMF C2 H F3 O2



RN 856188-44-8 HCAPLUS
CN Piperazine-3-13C-1-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

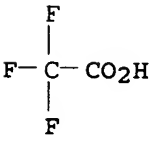
CM 1

CRN 856188-43-7
CMF C5 H12 N2



CM 2

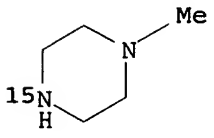
CRN 76-05-1
CMF C2 H F3 O2



RN 856188-50-6 HCAPLUS
CN Piperazine-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

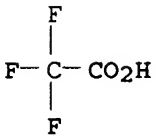
CM 1

CRN 856188-49-3
CMF C5 H12 N2

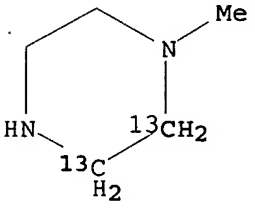


CM 2

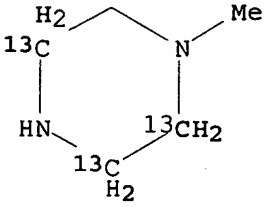
CRN 76-05-1
CMF C2 H F3 O2



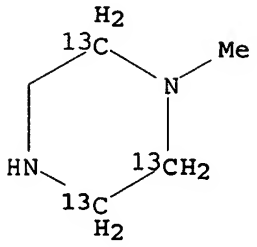
RN 857503-04-9 HCAPLUS
CN Piperazine-2,3-13C2, 1-methyl- (9CI) (CA INDEX NAME)



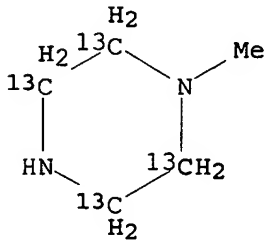
RN 857503-05-0 HCAPLUS
CN Piperazine-13C3, 1-methyl- (9CI) (CA INDEX NAME)



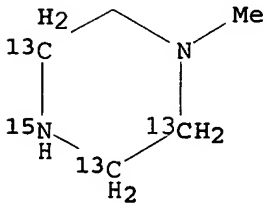
RN 857503-06-1 HCAPLUS
CN Piperazine-13C3, 4-methyl- (9CI) (CA INDEX NAME)



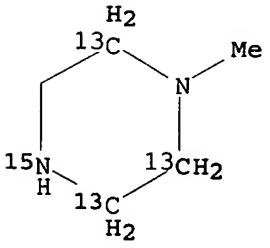
RN 857503-07-2 HCAPLUS
CN Piperazine-13C4, 1-methyl- (9CI) (CA INDEX NAME)



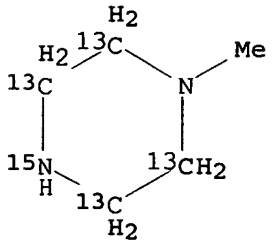
RN 857503-08-3 HCAPLUS
CN Piperazine-2,3,6-13C3-1-15N, 4-methyl- (9CI) (CA INDEX NAME)



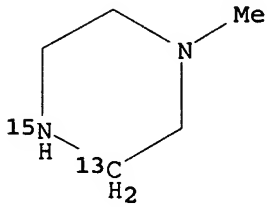
RN 857503-09-4 HCAPLUS
CN Piperazine-2,3,5-13C3-1-15N, 4-methyl- (9CI) (CA INDEX NAME)



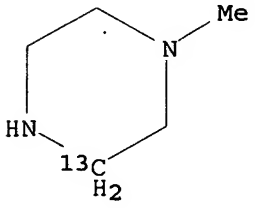
RN 857503-10-7 HCAPLUS
CN Piperazine-13C4-15N, 4-methyl- (9CI) (CA INDEX NAME)



RN 857503-11-8 HCAPLUS
CN Piperazine-2-13C-1-15N, 4-methyl- (9CI) (CA INDEX NAME)



RN 857503-12-9 HCAPLUS
CN Piperazine-13C, 4-methyl- (9CI) (CA INDEX NAME)



L42 ANSWER 4 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:592129 HCAPLUS
DN 143:97398
TI Preparation of active esters of N-substituted piperazine acetic acids, including **isotopically** enriched versions
IN Dey, Subhakar; Pappin, Darryl J. C.; Purkayastha, Subhasish; Pillai, Sasi; Coull, James M.
PA Applera Corp., USA
SO U.S. Pat. Appl. Publ., 33 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 6

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2005148771	A1	20050707	US 2004-751354	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105

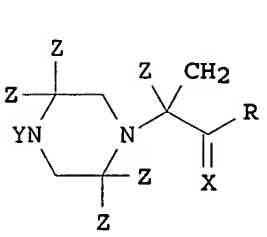
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

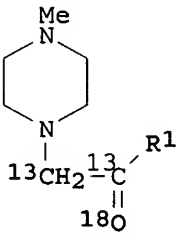
PRAI US 2004-751353 A 20040105
US 2004-751354 A 20040105
US 2004-751387 A 20040105
US 2004-751388 A 20040105
US 2004-822639 A 20040412
US 2004-852730 A 20040524

OS MARPAT 143:97398

GI



I



II

AB In some embodiments, this invention pertains to active esters of N-substituted piperazine acetic acid I (R = leaving group; X = O, S; Y = C1-C6 alkyl, C1-C6 alkyl ether; Z = H, 2H, F, Cl, Br, iodide, amino acid side chain, C1-C6 alkyl, C1-C6 alkyl ether), including **isotopically** enriched versions thereof. In some embodiments, this invention pertains to methods for the preparation of active esters of N-substituted piperazine acetic acid, including **isotopically** enriched versions thereof. For example, the **isotopically** labeled N-methylpiperazine II (R1 = 18OH) reacted with the trifluoroacetic acid ester of N-hydroxysuccinimide to give the succinate II (R1 = OR2, R2 = succinimido).

IC ICM C07D043-02
ICS C07D241-04

INCL 544182000; 544372000; 544209000; 544371000; 544399000

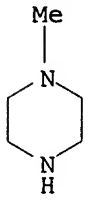
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

IT **109-01-3P**, N-Methylpiperazine 5625-52-5P 145590-97-2P
856187-53-6P **856187-57-0P** 856187-64-9P 856187-68-3P
856187-72-9P 856187-80-9P 856187-83-2P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

IT 856187-76-3P 856187-92-3P 856188-23-3P 856188-27-7P 856188-32-4P
856188-38-0P 856188-44-8P 856188-50-6P
856188-62-0P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

IT **109-01-3P**, N-Methylpiperazine **856187-57-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and

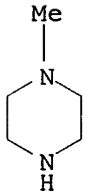
their labeled derivs.)
RN 109-01-3 HCAPLUS
CN Piperazine, 1-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 856187-57-0 HCAPLUS
CN Piperazine, 1-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

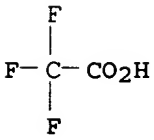
CM 1

CRN 109-01-3
CMF C5 H12 N2



CM 2

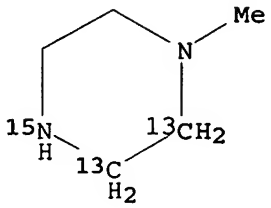
CRN 76-05-1
CMF C2 H F3 O2



IT **856188-38-0P 856188-44-8P 856188-50-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)
RN 856188-38-0 HCAPLUS
CN Piperazine-2,3-13C2-1-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

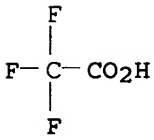
CM 1

CRN 856188-37-9
CMF C5 H12 N2



CM 2

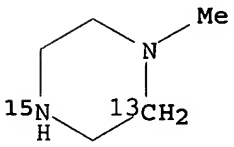
CRN 76-05-1
CMF C2 H F3 O2



RN 856188-44-8 HCAPLUS
CN Piperazine-3-13C-1-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

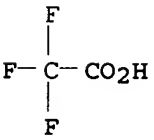
CM 1

CRN 856188-43-7
CMF C5 H12 N2



CM 2

CRN 76-05-1
CMF C2 H F3 O2

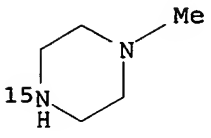


RN 856188-50-6 HCAPLUS
CN Piperazine-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

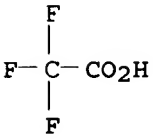
CRN 856188-49-3

CMF C5 H12 N2



CM 2

CRN 76-05-1
CMF C2 H F3 O2



L42 ANSWER 5 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:592027 HCAPLUS
DN 143:93642
TI Mixtures of isobarically labeled analytes and fragments ions derived therefrom
IN Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.
PA Applera Corp., USA
SO U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. Ser. No. 751,353.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005147985	A1	20050707	US 2004-822639	20040412
	US 2005147982	A1	20050707	US 2004-751353	20040105
	US 2005148087	A1	20050707	US 2004-852730	20040524
	WO 2005068446	A1	20050728	WO 2005-US223	20050105
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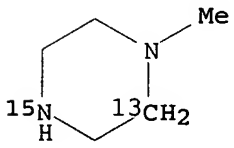
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2004-751353	A2	20040105		
	US 2004-751354	A	20040105		
	US 2004-751387	A	20040105		
	US 2004-751388	A	20040105		
	US 2004-822639	A2	20040412		
	US 2004-852730	A	20040524		

OS MARPAT 143:93642
AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.
IC ICM C12Q001-68
ICS C07H021-02; G01N033-00; C07J043-00
INCL 435006000; 436086000; 530409000; 536023100; 540107000; 544359000
CC 9-16 (Biochemical Methods)
IT 856188-23-3P 856188-27-7P 856188-32-4P 856188-38-0P
856188-44-8P 856188-50-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)
IT **856188-44-8P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)
RN 856188-44-8 HCAPLUS
CN Piperazine-3-13C-1-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 856188-43-7
CMF C5 H12 N2



CM 2

CRN 76-05-1
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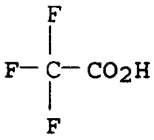


L42 ANSWER 6 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:588426 HCAPLUS
DN 143:115568
TI Preparation of **isotopically** enriched N-substituted piperazine-1-acetic acids
IN Dey, Subhakar; Pappin, Darryl J. c.; Purkayastha, Subhasish; Pillai, Sasi; Coull, James M.
PA Applera Corp., USA
SO U.S. Pat. Appl. Publ., 29 pp.
CODEN: USXXCO

DT Patent
LA English
FAN.CNT 6

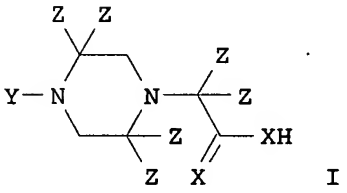
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005148774	A1	20050707	US 2004-751387	20040105
	WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI	US 2004-751353	A	20040105
	US 2004-751354	A	20040105
	US 2004-751387	A	20040105
	US 2004-751388	A	20040105
	US 2004-822639	A	20040412
	US 2004-852730	A	20040524

OS MARPAT 143:115568
GI



I

AB **Isotopically** enriched N-substituted piperazine-1-acetic acids (I) or salts thereof, comprising one or more heavy atom **isotopes** [X = O, S; Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or F atoms; Z = independently H, deuterium, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms), a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms, or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms)] are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to

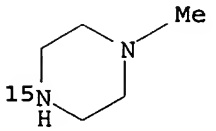
label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like. Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

IC ICM C07D241-04
INCL 544399000
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 6, 80
ST **isotopically** enriched methylpiperazine prepn isobaric labeling reagent; methylpiperazineacetic acid **isotope** labeled prepn isobaric labeling reagent
IT **Isotope** indicators
(preparation of **isotopically** enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
IT 856188-20-0P
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of **isotopically** enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
IT 79-08-3, Bromoacetic acid 87-86-5, Pentachlorophenol 109-01-3, N-Methylpiperazine 407-25-0, Trifluoroacetic anhydride 554-84-7, 3-Nitrophenol 658-78-6, Trifluoroacetic acid p-nitrophenyl ester 920-66-1, 1,1,1,3,3,3-Hexafluoropropan-2-ol 1737-40-2, Trifluoroacetic acid 3-nitrophenyl ester 6066-82-6, N-Hydroxysuccinimide 13200-60-7, Sarcosine ethyl ester 14314-42-2, Water-18O 14533-84-7, Trifluoroacetic acid pentafluorophenyl ester 18156-74-6, 1-Trimethylsilylimidazole 28230-32-2 52928-63-9, N-Hydroxy-2-pyrrolidinone 56522-24-8, tert-Butyldimethylsilyl cyanide 61898-49-5 85539-84-0 856187-95-6, 4-Methylpiperazine-1-acetic acid phenyl ester 857291-01-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of **isotopically** enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
IT 79-08-3DP, Bromoacetic acid, trityl chloride resin-bound 5672-86-6P, Trifluoroacetic acid pentachlorophenyl ester 5672-89-9P, Trifluoroacetic acid succinimidyl ester 54699-92-2P, 4-Methylpiperazine-1-acetic acid 145142-92-3P 145142-94-5P 856187-64-9P 856187-68-3P 856187-72-9P 856187-80-9P 856187-83-2P 856188-16-4P 856188-80-2P 856188-88-0P, Trifluoroacetic acid 2-oxopyrrolidin-1-yl ester 857027-04-4P 857027-05-5P 857027-07-7P 857502-95-5P 857502-96-6P 857502-97-7P 857502-98-8P **857502-99-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of **isotopically** enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
IT 856187-76-3P 856187-87-6P 856187-92-3P 856188-02-8P, 4-Methylpiperazine-1-acetic acid 1,1,1,3,3,3-hexafluoropropan-2-yl ester 856188-06-2P 856188-23-3P 856188-27-7P 856188-32-4P **856188-37-9P 856188-38-0P 856188-43-7P 856188-44-8P 856188-49-3P 856188-50-6P** 856188-62-0P 856290-53-4P 856290-55-6P 857027-09-9P 857027-10-2P 857027-11-3P 857027-12-4P 857503-00-5P 857503-01-6P 857503-02-7P

857503-03-8P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of **isotopically** enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

IT **857502-99-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of **isotopically** enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

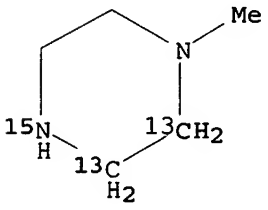
RN 857502-99-9 HCAPLUS
CN Piperazine-15N, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

IT **856188-37-9P 856188-38-0P 856188-43-7P**
856188-44-8P 856188-49-3P 856188-50-6P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of **isotopically** enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

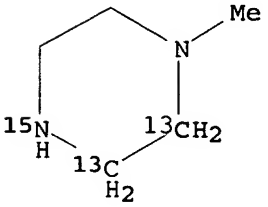
RN 856188-37-9 HCAPLUS
CN Piperazine-2,3-13C2-1-15N, 4-methyl- (9CI) (CA INDEX NAME)



RN 856188-38-0 HCAPLUS
CN Piperazine-2,3-13C2-1-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

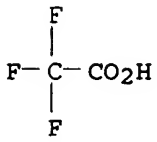
CM 1

CRN 856188-37-9
CMF C5 H12 N2

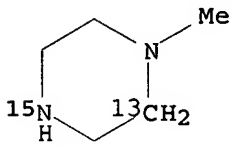


CM 2

CRN 76-05-1
CMF C2 H F3 O2



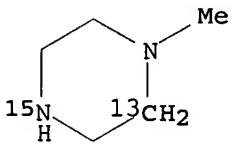
RN 856188-43-7 HCAPLUS
CN Piperazine-3-13C-1-15N, 4-methyl- (9CI) (CA INDEX NAME)



RN 856188-44-8 HCAPLUS
CN Piperazine-3-13C-1-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

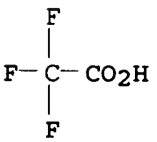
CM 1

CRN 856188-43-7
CMF C5 H12 N2

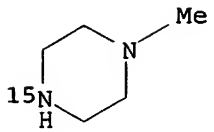


CM 2

CRN 76-05-1
CMF C2 H F3 O2



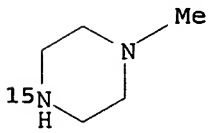
RN 856188-49-3 HCAPLUS
CN Piperazine-15N, 4-methyl- (9CI) (CA INDEX NAME)



RN 856188-50-6 HCAPLUS
CN Piperazine-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 856188-49-3
CMF C5 H12 N2



CM 2

CRN 76-05-1
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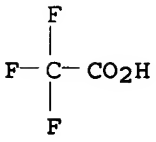

L42 ANSWER 7 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:588349 HCAPLUS
DN 143:112150
TI Isobarically labeled analytes and fragment ions derived therefrom
IN Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.
PA Applera Corporation, USA
SO U.S. Pat. Appl. Publ., 88 pp., Cont.-in-part of U.S. Ser. No. 822,639.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 6

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2005148087	A1	20050707	US 2004-852730	20040524
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005147985	A1	20050707	US 2004-822639	20040412
WO 2005068446	A1	20050728	WO 2005-US223	20050105

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NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

PRAI US 2004-751353 A2 20040105
US 2004-822639 A2 20040412
US 2004-751354 A 20040105
US 2004-751387 A 20040105
US 2004-751388 A 20040105
US 2004-852730 A 20040524

OS MARPAT 143:112150

AB This invention pertains to isobarically labeled analytes and fragment ions thereof.

IC ICM C07K014-47
ICS C12Q001-68; G01N033-00

INCL 436086000; 530409000

CC 9-16 (Biochemical Methods)

IT 856188-27-7P 856188-32-4P 856188-38-0P **856188-44-8P**
856188-50-6P 857290-86-9P
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(isobarically labeled analytes and fragment ions derived therefrom)

IT 79-08-3DP, Bromoacetic acid, polystyrene trityl chloride piperazine derivs. 110-85-0DP, Piperazine, trityl chloride/bromoacetic polystyrene derivs. 3235-67-4P, 1-Piperidineacetic acid 3235-69-6P, 4-Morpholineacetic acid 5625-52-5P 37478-58-3P, 1-Piperazineacetic acid 53788-49-1P 80841-13-0P 174311-10-5P 215101-76-1P 741683-82-9P, 1-Piperidineacetic-carboxy-13C acid 741683-83-0P, 1-Piperidineacetic-α-13C acid **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid **741683-85-2P**, 1-Piperazineacetic-α-13C acid 856187-64-9P 856187-72-9P 856187-80-9P 856187-83-2P 857027-04-4P 857027-05-5P 857027-07-7P 857027-09-9P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(isobarically labeled analytes and fragment ions derived therefrom)

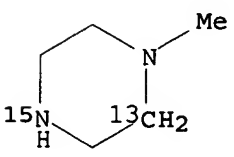
IT **856188-44-8P**
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(isobarically labeled analytes and fragment ions derived therefrom)

RN 856188-44-8 HCAPLUS

CN Piperazine-3-13C-1-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

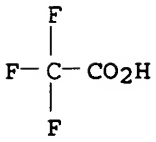
CM 1

CRN 856188-43-7
CMF C5 H12 N2

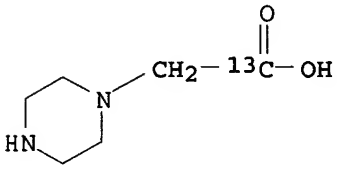


CM 2

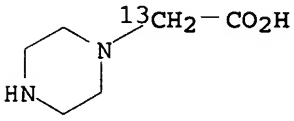
CRN 76-05-1
CMF C2 H F3 O2



IT **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid
741683-85-2P, 1-Piperazineacetic-α-13C acid
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(isobarically labeled analytes and fragment ions derived therefrom)
RN 741683-84-1 HCAPLUS
CN 1-Piperazineacetic-carboxy-13C acid (9CI) (CA INDEX NAME)



RN 741683-85-2 HCAPLUS
CN 1-Piperazineacetic-α-13C acid (9CI) (CA INDEX NAME)



L42 ANSWER 8 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:588336 HCAPLUS
DN 143:93635
TI Mixtures of isobarically labeled analytes and fragments ions derived therefrom
IN Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.
PA Applera Corporation, USA
SO U.S. Pat. Appl. Publ., 29 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005147982	A1	20050707	US 2004-751353	20040105
	US 2005147985	A1	20050707	US 2004-822639	20040412
	US 2005148087	A1	20050707	US 2004-852730	20040524
	WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2004-751353 A2 20040105
US 2004-751354 A 20040105
US 2004-751387 A 20040105
US 2004-751388 A 20040105
US 2004-822639 A2 20040412
US 2004-852730 A 20040524

AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.

IC ICM C12Q001-68
ICS C07H021-04; G01N033-00; C07K014-47

INCL 435006000; 436086000; 530409000; 536023100

CC 9-16 (Biochemical Methods)

IT 856188-38-0P **856188-44-8P**
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

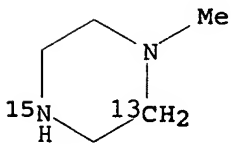
IT **856188-44-8P**
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856188-44-8 HCAPLUS

CN Piperazine-3-13C-1-15N, 4-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

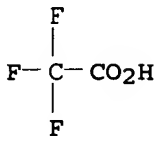
CM 1

CRN 856188-43-7
CMF C5 H12 N2

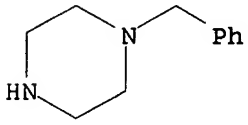


CM 2

CRN 76-05-1
CMF C2 H F3 O2



L42 ANSWER 9 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:460973 HCAPLUS
DN 143:152841
TI One-step exchange-labeling of piperidines, piperazines and dialkylamines with deuterium oxide: catalysis by various ruthenium complexes
AU Alexakis, Efstathios; Hickey, Michael J.; Jones, John R.; Kingston, Lee P.; Lockley, William J. S.; Mather, Andrew N.; Smith, Traci; Wilkinson, David J.
CS School of Biomedical and Molecular Sciences, Department of Chemistry, University of Surrey, Surrey, Guildford, GU2 7XH, UK
SO Tetrahedron Letters (2005), 46(25), 4291-4293
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 143:152841
AB A range of variously substituted piperidines, piperazines, and dialkylamines can be conveniently deuterated in a single step by **isotopic** exchange with deuterium oxide in the presence of an appropriate ruthenium complex catalyst. The **isotopic** exchange can be carried out efficiently in DMSO; hence it is directly applicable to the deuteration of polar compds. such as pharmaceuticals. **Isotopic** incorporations are high, while recoveries are variable and generally moderate. Deuteration takes place at positions both α and β to the NH group.
CC 21-2 (General Organic Chemistry)
IT 859843-14-4P 860027-49-2P **860027-50-5P** 860027-51-6P
860027-52-7P 860027-53-8P 860027-54-9P 860027-55-0P 860027-56-1P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(one-step exchange-labeling of piperidines, piperazines, and dialkylamines with deuterium oxide catalyzed by ruthenium complexes)
IT **860027-50-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(one-step exchange-labeling of piperidines, piperazines, and dialkylamines with deuterium oxide catalyzed by ruthenium complexes)
RN 860027-50-5 HCAPLUS
CN Piperazine, 1-(phenylmethyl)-, labeled with deuterium (9CI) (CA INDEX NAME)

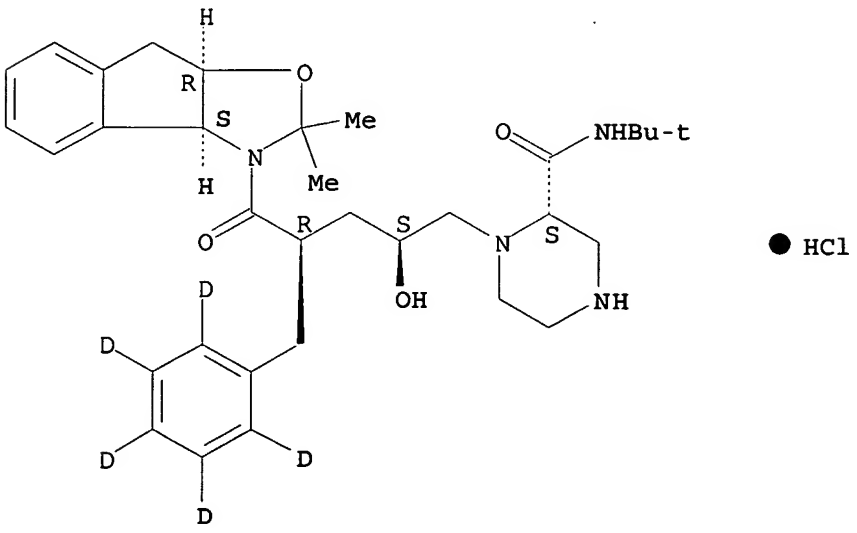


RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 10 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:284712 HCAPLUS

DN 144:7060
TI **Isotope** labeled 'HEA/HEE' moiety in the synthesis of labeled HIV-protease inhibitors. Part II
AU Ekhato, I. Victor; Liao, Yuan; Plesescu, Mihaela
CS Pharmaceutical Research Institute, Bristol-Myers Squibb Company, Wallingford, CT, 06492, USA
SO Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(3), 179-193
CODEN: JLCRD4; ISSN: 0362-4803
PB John Wiley & Sons Ltd.
DT Journal
LA English
AB [2H5]-Amprenavir and [2H5]-saquinavir were prepared from a common labeled precursor, tert-Bu (1S,2S)-(1-oxiranyl-2-[2H5]phenylethyl)carbamate. Both of these compds. are in the 'HEA' class of HIV protease inhibitors. [2H5]-Indinavir, a representative of the 'HEE' group of protease inhibitors, was also synthesized. In the case of indinavir, 1S-(2,2-dimethyl-8,8a-dihydro-3aH-indeno[1,2-d]oxazol-3R-yl)-2-oxiranylmethyl-3-[2H5]phenylpropan-1-one provided the [phenyl-2H5]-HEE core structure for synthesis of the desired labeled compound
CC 34-3 (Amino Acids, Peptides, and Proteins)
IT 870073-14-6P 870073-15-7P 870073-16-8P 870073-17-9P 870073-18-0P 870073-19-1P 870073-22-6P **870073-23-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of deuterium-labeled amprenavir, saquinavir, and indinavir)
IT **870073-23-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of deuterium-labeled amprenavir, saquinavir, and indinavir)
RN 870073-23-7 HCAPLUS
CN 2H-Indeno[1,2-d]oxazole, 3,3a,8,8a-tetrahydro-2,2-dimethyl-3-[2,3,5-trideoxy-5-[(2S)-2-[[(1,1-dimethylethyl)amino]carbonyl]-1-piperazinyl]-2-(phenyl-d5-methyl)-D-erythro-pentonoyl]-, monohydrochloride, (3aS,8aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 11 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:76240 HCAPLUS
DN 142:176839
TI Preparation of heterocycloalkylmethylimidazoles and related compounds as C5a receptor modulators for the treatment of inflammatory disorders
IN Zhang, Suoming; He, Zhao; Gao, Yang; Thurkauf, Andrew; Maynard, George; Bertrand, Chenard; Ohliger, Robert; Peterson, John M.
PA Neurogen Corporation, USA
SO PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005007087	A2	20050127	WO 2004-US21191	20040630
	WO 2005007087	A3	20060330		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2006154917	A1	20060713	US 2006-563401	20060103
PRAI	US 2003-484684P	P	20030703		
	WO 2004-US21191	W	20040630		

OS MARPAT 142:176839
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A = O, S, NR; X = J; Y = K; Z = (L)m; Q = Ar1; m = 0-2; J, K, L = O, S, NH, etc. with provisos; R = alkyl, alkenyl, alkynyl, etc.; R1 = H, OH, halo, etc.; R2, R3 = H, alkyl; R4 = alkyl, alkenyl, alkynyl, etc.; R5 = OH, halo, amino, etc. with provisos; Ar1 = (un)substituted Ph, naphthyl, heteroaryl, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, N-alkylation of 2-benzo[1,3]dioxol-5-ylpiperidine with chloride II, e.g., prepared from 4,5-dichloroimidazole in 6-steps, afforded methylimidazole III. Compds. I are claimed to be modulators of C5a receptors, preferably bind to C5a receptors with high affinity and exhibit neutral antagonist or inverse agonist activity at C5a receptors.

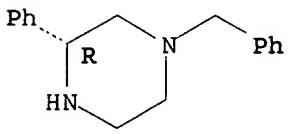
IC ICM A61K
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
IT **Isotopomers**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of heterocycloalkylmethylimidazoles and related compds. as C5a receptor modulators for the treatment of inflammatory disorders)
IT 7238-61-1P, 2-Bromo-4-methylthiazole 31250-75-6P, 2,4,5-Tribromo-1-ethyl-

1H-imidazole 176961-50-5P, 2-Bromo-4-phenyloxazole 666834-27-1P, 2-Bromo-1-butyl-4,5-dichloro-1H-imidazole 832154-99-1P, 1-Butyl-4,5-dichloro-1H-imidazole 832155-00-7P 832155-01-8P, 3-Butyl-5-chloro-2-(2,6-dimethylphenyl)-3H-imidazole-4-carboxaldehyde 832155-02-9P, [3-Butyl-5-chloro-2-(2,6-dimethylphenyl)-3H-imidazol-4-yl]methanol 832155-03-0P, 2-Methoxy-4-pyridin-2-ylbenzoic acid methyl ester 832155-04-1P, 2-Methoxy-4-piperidin-2-ylbenzoic acid methyl ester 832155-05-2P 832155-06-3P 832155-07-4P 832155-08-5P, 4,5-Dibromo-2-(2,6-diethylphenyl)-1-ethyl-1H-imidazole **832155-10-9P**, (R)-1-Benzyl-3-phenylpiperazine 832155-11-0P, 2-(2,6-Diethylphenyl)-4-methylthiazole 832155-12-1P, 5-Bromo-2-(2,6-diethylphenyl)-4-methylthiazole 832155-13-2P, 2-(2,6-Diethylphenyl)-4-methylthiazole-5-carboxaldehyde 832155-14-3P, [2-(2,6-Diethylphenyl)-4-methylthiazol-5-yl]methanol 832155-15-4P, 2-(2,6-Diethylphenyl)-4-phenyloxazole 832155-16-5P, 5-Bromo-2-(2,6-diethylphenyl)-4-phenyloxazole 832155-17-6P, 2-(2,6-Diethylphenyl)-4-phenyloxazole-5-carboxaldehyde 832155-18-7P, [2-(2,6-Diethylphenyl)-4-phenyloxazol-5-yl]methanol
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of heterocycloalkylmethylimidazoles and related compds. as C5a receptor modulators for the treatment of inflammatory disorders)

IT **832155-10-9P**, (R)-1-Benzyl-3-phenylpiperazine
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of heterocycloalkylmethylimidazoles and related compds. as C5a receptor modulators for the treatment of inflammatory disorders)

RN 832155-10-9 HCAPLUS
CN Piperazine, 3-phenyl-1-(phenylmethyl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L42 ANSWER 12 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:1087089 HCAPLUS
DN 142:190130
TI Automated 96-well solid phase extraction and hydrophilic interaction liquid chromatography-tandem mass spectrometric method for the analysis of cetirizine (ZYRTEC) in human plasma-with emphasis on method ruggedness
AU Song, Qi; Junga, Heiko; Tang, Yong; Li, Austin C.; Addison, Tom; McCort-Tipton, Melanie; Beato, Brian; Weng, Naidong
CS LLC, Covance Bioanalytical Services, Indianapolis, IN, 46214, USA
SO Journal of Chromatography, B: Analytical Technologies in the Biomedical and Life Sciences (2005), 814(1), 105-114
CODEN: JCBAAI; ISSN: 1570-0232
PB Elsevier B.V.
DT Journal
LA English
AB A high-throughput bioanal. method based on automated sample transfer, automated solid phase extraction, and hydrophilic interaction liquid chromatog.-tandem mass spectrometry (HILIC-MS/MS) anal., has been developed for the determination of cetirizine, a selective H1-receptor antagonist.

Deuterated cetirizine (cetirizine-d8) was synthesized as described and was used as the internal standard Samples were transferred into 96-well plates using an automated sample handling system. Automated solid phase extraction was carried out using a 96-channel programmable liquid-handling workstation. Solid phase extraction 96-well plate on polymer sorbent (Strata X) was used to extract the analyte. The extracted samples were injected onto a Betasil silica column (50 + 3, 5 μm) using a mobile phase of acetonitrile-water-acetic acid-trifluroacetic acid (93:7:1:0.025, volume/volume/volume/volume) at a flow rate of 0.5 mL/min. The chromatog. run time is 2.0 min per injection, with retention time of cetirizine and cetirizine-d8 both at 1.1 min. The system consisted of a Shimadzu HPLC system and a PE Sciex API 3000 or API 4000 tandem mass spectrometer with (+) ESI. The method has been validated over the concentration range of 1.00-1000 ng/mL cetirizine in human plasma, based on a 0.10-mL sample size. The interday precision and accuracy of the quality control (QC) samples demonstrated <3.0% relative standard deviation (R.S.D.) and <6.0% relative error (RE). Stability of cetirizine in stock solution, in plasma, and in reconstitution solution was established. The absolute extraction recovery was 85.8%, 84.5%, and 88.0% at 3, 40, and 800 ng/mL, resp. The recovery for the internal standard was 84.1%. No adverse matrix effects were noticed for this assay. The automation of the sample preparation steps not only increased the anal. throughput, but also increased method ruggedness. The use of a stable **isotope**-labeled internal standard further improved the method ruggedness. Practical issues of analyzing incurred samples were discussed. This HILIC-MS/MS method for anal. of citirizine in human plasma was successfully used to support clin. studies.

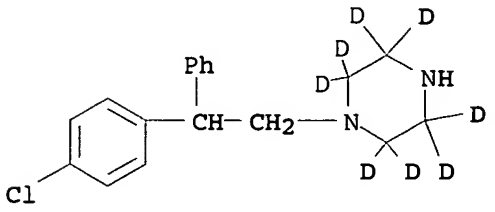
CC 1-1 (Pharmacology)

IT 36961-64-5P, 2-Chloroethoxy acetamide **838818-78-3P** 838818-79-4P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(automated 96-well solid phase extraction and hydrophilic interaction liquid chromatog.-tandem mass spectrometric method for anal. of cetirizine (ZYRTEC) in human plasma-with emphasis on method ruggedness)

IT **838818-78-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(automated 96-well solid phase extraction and hydrophilic interaction liquid chromatog.-tandem mass spectrometric method for anal. of cetirizine (ZYRTEC) in human plasma-with emphasis on method ruggedness)

RN 838818-78-3 HCAPLUS

CN Piperazine-2,2,3,3,5,5,6,6-d8, 1-[2-(4-chlorophenyl)-2-phenylethyl]- (9CI) (CA INDEX NAME)



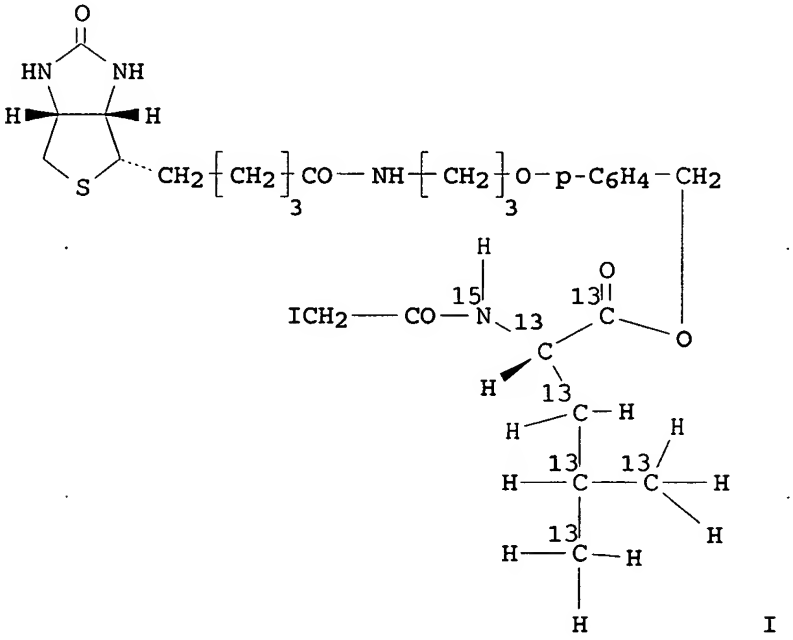
RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 13 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:992678 HCAPLUS
DN 141:411222
TI Synthesis of **isotope**-coded affinity tags and their use for protein anal. using solid-phase or solution chemical techniques
IN Auriel, Daniel; Immler, Dorian; Lerchen, Hans-Georg; Schumacher, Andreas
PA Bayer HealthCare AG, Germany
SO Ger. Offen., 37 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 10319611	A1	20041118	DE 2003-10319611	20030502
PRAI DE 2003-10319611		20030502		

OS MARPAT 141:411222
GI

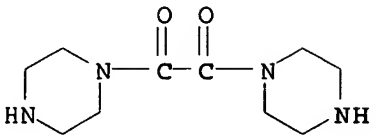


I

AB The invention concerns new, **isotope**-coded affinity markers, e.g., (I), for the mass-spectrometric anal. of proteins, as well as their production, their use, and kits containing them. Preparation of a 13C4-labeled piperazine ring, which can be incorporated in place of the benzene ring in these compds., was also given, beginning from Boc-glycine-13C2-OH. Title compds. were prepared with labels, e.g. biotin as shown, or with a solid-support in place of the label (claimed, no data). Thus, N-(3-bromopropyl)phthalimide was reacted with 4-hydroxybenzaldehyde, and the aldehyde group reduced to the alc., which was amine-deprotected and biotinylated, followed by esterification using labeled Fmoc-L-leucine; after deprotection, the resulting intermediate was acylated using iodoacetic anhydride.

IC ICM C07D495-04

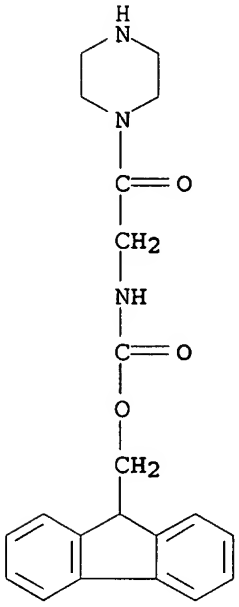
ICS G01N033-483
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 28, 63
ST affinity tag **isotope** prepn protein peptide mass spectral analysis
IT Affinity labeling
Mass spectra
(preparation of **isotope**-coded affinity tags and their use for protein anal. using solid-phase or solution chemical techniques)
IT Peptides, analysis
Proteins
RL: ANT (Analyte); ANST (Analytical study)
(preparation of **isotope**-coded affinity tags and their use for protein anal. using solid-phase or solution chemical techniques)
IT Heterocyclic compounds
RL: DGN (Diagnostic use); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of **isotope**-coded affinity tags and their use for protein anal. using solid-phase or solution chemical techniques)
IT 525587-15-9P 525587-16-0P 793682-22-1P 793682-23-2P 793682-24-3P
793682-25-4P 793682-26-5P 793682-27-6P 793682-28-7P 793682-29-8P
RL: DGN (Diagnostic use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of **isotope**-coded affinity tags and their use for protein anal. using solid-phase or solution chemical techniques)
IT 58-85-5, Biotin 79-37-8, Oxalyl chloride 121-33-5 123-08-0
1676-90-0 3303-84-2 3392-10-7 4530-20-5 5460-29-7 7536-55-2
13726-84-6 13734-41-3 18278-34-7 22838-58-0 25616-02-8
29022-11-5, Fmoc-gly-oh 31972-52-8 35661-60-0 54907-61-8, Iodoacetic acid anhydride 57078-98-5 57260-71-6 145142-99-0 219312-89-7
793682-02-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of **isotope**-coded affinity tags and their use for protein anal. using solid-phase or solution chemical techniques)
IT 73279-02-4P **105807-56-5P** 116753-56-1P 352359-09-2P
525586-90-7P 525586-91-8P 525586-92-9P 525586-93-0P,
Piperazine-13C4 525587-01-3P 525587-02-4P 525587-03-5P
525587-06-8P 525587-07-9P 525587-08-0P 525587-09-1P 525587-10-4P
525587-11-5P 525587-12-6P 525587-13-7P 525587-34-2P 525587-35-3P
525587-37-5P, 2,5-Piperazinedione-2,3,5,6-13C4 525587-39-7P
525587-40-0P 525587-42-2P 525587-44-4P 525587-89-7P
525587-91-1P 773871-63-9P 793682-03-8P 793682-04-9P 793682-05-0P
793682-06-1P 793682-07-2P 793682-08-3P 793682-09-4P 793682-10-7P
793682-11-8P 793682-12-9P 793682-13-0P **793682-14-1P**
793682-15-2P 793682-16-3P 793682-17-4P 793682-18-5P
793682-19-6P 793682-20-9P 793682-21-0P 793682-30-1P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of **isotope**-coded affinity tags and their use for protein anal. using solid-phase or solution chemical techniques)
IT **105807-56-5P 525586-90-7P 525587-40-0P**
793682-14-1P 793682-19-6P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of **isotope**-coded affinity tags and their use for protein anal. using solid-phase or solution chemical techniques)
RN 105807-56-5 HCAPLUS
CN Piperazine, 1,1'-(1,2-dioxo-1,2-ethanediyl)bis- (9CI) (CA INDEX NAME)



RN 525586-90-7 HCAPLUS
CN Carbamic acid, [2-oxo-2-(1-piperazinyl)ethyl]-, 9H-fluoren-9-ylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

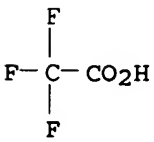
CM 1

CRN 525586-89-4
CMF C21 H23 N3 O3

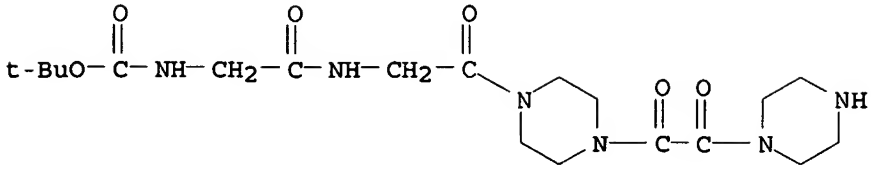


CM 2

CRN 76-05-1
CMF C2 H F3 O2

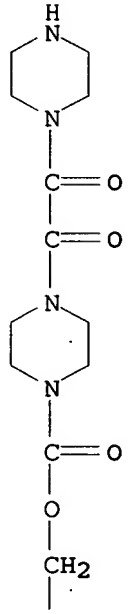


RN 525587-40-0 HCAPLUS
CN Carbamic acid, [2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinylacetyl)-1-piperazinyl]ethyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

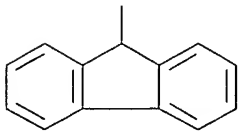


RN 793682-14-1 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-(oxo-1-piperazinylacetyl)-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



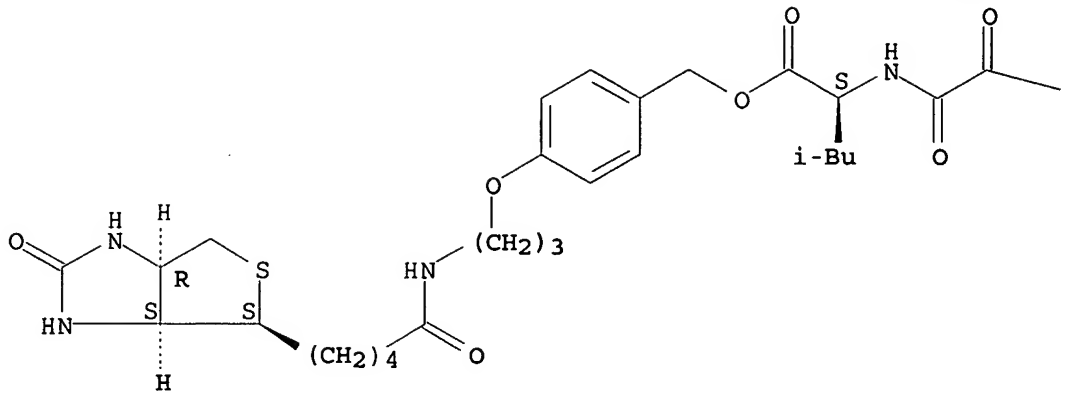
PAGE 2-A



RN 793682-19-6 HCAPLUS
CN L-Leucine, N-[oxo[4-(oxo-1-piperazinylacetyl)-1-piperazinyl]acetyl]-, [4-[3-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]propoxy]phenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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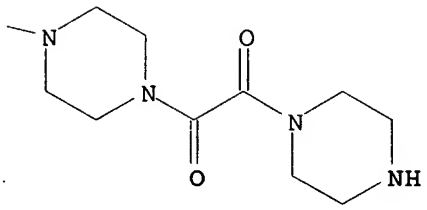


L42 ANSWER 14 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:859475 HCAPLUS
DN 143:26320
TI Synthesis of [3,5-dichlorobenzenesulfonamide-U-14C)] labeled VLA-4 antagonists
AU Yu, Nathan X.; Raab, Conrad E.; Dean, Dennis C.; Melillo, David G.
CS Department of Drug Metabolism, Merck & Co., Inc., Rahway, NJ, 07065, USA
SO Synthesis and Applications of Isotopically Labelled Compounds, Proceedings of the International Symposium, 8th, Boston, MA, United States, June 1-5, 2003 (2004), Meeting Date 2003, 429-432. Editor(s): Dean, Dennis C.; Filer, Crist N.; McCarthy, Keith E. Publisher: John Wiley & Sons Ltd., Chichester, UK.
CODEN: 69FZAZ; ISBN: 0-470-86365-X
DT Conference
LA English
OS CASREACT 143:26320
AB Radiolabeled tracers were required for the development of a series of VLA-4 antagonists. A method to synthesize [U-14C]3,5-dichlorobenzenesulfonyl chloride was developed. From this key intermediate, various tracers were prepared in high yield.
CC 25-13 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 74
IT **Isotope** indicators
(preparation of 14C-labeled (dichlorophenylsulfonyl)azetidinecarboxamides as radiotracers via amidation of azetidinecarboxamides with 14C-labeled dichlorophenylsulfonyl chloride followed by hydrolysis)

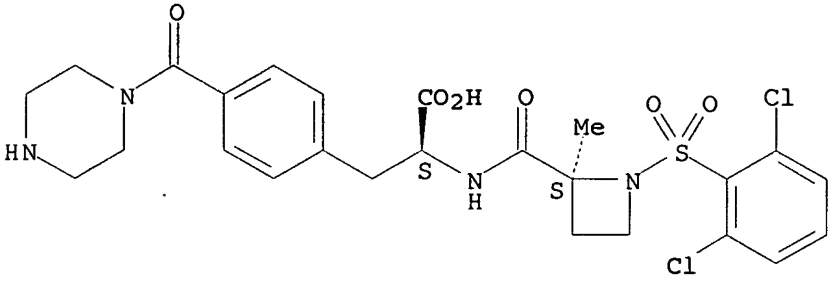
IT **Isotopomers**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 14C-labeled (dichlorophenylsulfonyl)azetidinecarboxamides as radiotracers via amidation of azetidinecarboxamides with 14C-labeled dichlorophenylsulfonyl chloride followed by hydrolysis)

IT **757977-77-8P 757977-78-9P 757977-79-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of 14C-labeled (dichlorophenylsulfonyl)azetidinecarboxamides as radiotracers via amidation of azetidinecarboxamides with 14C-labeled dichlorophenylsulfonyl chloride followed by hydrolysis and deprotection)

IT **757977-77-8P 757977-78-9P 757977-79-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of 14C-labeled (dichlorophenylsulfonyl)azetidinecarboxamides as radiotracers via amidation of azetidinecarboxamides with 14C-labeled dichlorophenylsulfonyl chloride followed by hydrolysis and deprotection)

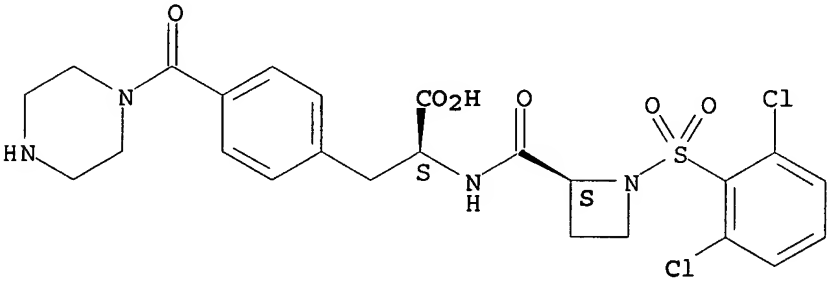
RN 757977-77-8 HCAPLUS
CN L-Phenylalanine, N-[[(2S)-1-[(2,6-dichlorophenyl)sulfonyl]-2-methyl-2-azetidinyl]carbonyl]-4-(1-piperazinylcarbonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



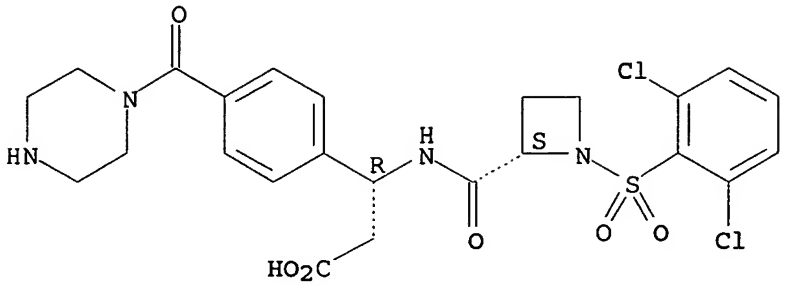
RN 757977-78-9 HCAPLUS
CN L-Phenylalanine, N-[[(2S)-1-[(2,6-dichlorophenyl)sulfonyl]-2-azetidinyl]carbonyl]-4-(1-piperazinylcarbonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 757977-79-0 HCAPLUS
CN Benzenepropanoic acid, β-[[[(2S)-1-[(2,6-dichlorophenyl)sulfonyl]-2-azetidinyl]carbonyl]amino]-4-(1-piperazinylcarbonyl)-, labeled with carbon-14, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 15 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:681717 HCAPLUS
DN 141:202794
TI Methods, mixtures, kits and compositions pertaining to analyte determination
IN Pappin, Darryl J. C.; Bartlet-Jones, Michael
PA Applera Corporation, USA
SO PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

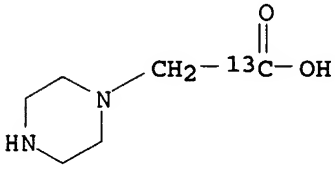
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004070352	A2	20040819	WO 2004-US2077	20040127
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004209401	A1	20040819	AU 2004-209401	20040127
	CA 2488584	AA	20040819	CA 2004-2488584	20040127
	US 2004219685	A1	20041104	US 2004-765264	20040127
	US 2004220412	A1	20041104	US 2004-765267	20040127
	US 2004219686	A1	20041104	US 2004-765458	20040127
	EP 1588145	A2	20051026	EP 2004-705571	20040127
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	US 2006105416	A1	20060518	US 2005-319685	20051228
PRAI	US 2003-443612P	P	20030130		
	US 2004-765267	A1	20040127		
	WO 2004-US2077	W	20040127		

AB This invention pertains to methods, mixts., kits and/or compns. for the determination of analytes by mass anal. using unique labeling reagents or sets of unique labeling reagents. The labeling reagents can be isomeric or isobaric and can be used to produce mixts. suitable for multiplex anal. of the labeled analytes.
IC ICM G01N
CC 9-16 (Biochemical Methods)
IT 3235-67-4P, 1-Piperidineacetic acid 3235-69-6P, 4-Morpholineacetic acid 37478-58-3P, 1-Piperazineacetic acid 215101-76-1P 741683-82-9P,

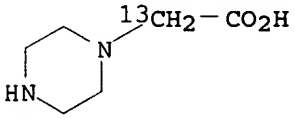
1-Piperidineacetic-carboxy-13C acid 741683-83-0P, 1-Piperidineacetic-α-13C acid **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid **741683-85-2P**, 1-Piperazineacetic-α-13C acid 741683-87-4P, 4-Morpholineacetic-carboxy-13C acid 741683-88-5P, 4-Morpholineacetic-α-13C acid
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(methods, mixts., kits and compns. pertaining to analyte determination)

IT **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid
741683-85-2P, 1-Piperazineacetic-α-13C acid
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(methods, mixts., kits and compns. pertaining to analyte determination)

RN 741683-84-1 HCAPLUS
CN 1-Piperazineacetic-carboxy-13C acid (9CI) (CA INDEX NAME)



RN 741683-85-2 HCAPLUS
CN 1-Piperazineacetic-α-13C acid (9CI) (CA INDEX NAME)



L42 ANSWER 16 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:306373 HCAPLUS
DN 140:316592
TI Preparation of nodulisporic acid derivatives as spot-on ectoparasiticides
IN Soll, Mark D.; Boeckh, Albert; De Bode, Ronus; Van Eijk, Peter Johannes Sevaas Savio
PA Merial Limited, USA
SO PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004030457	A1	20040415	WO 2003-US30500	20030929

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,

	BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004077703	A1	20040422	US 2003-618975	20030714
	CA 2500822	AA	20040415	CA 2003-2500822	20030929
	AU 2003279002	A1	20040423	AU 2003-279002	20030929
	EP 1545211	A1	20050629	EP 2003-770513	20030929
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	BR 2003014531	A	20050809	BR 2003-14531	20030929
	CN 1700859	A	20051123	CN 2003-825307	20030929
	JP 2006502241	T2	20060119	JP 2005-500323	20030929
	ZA 2005002904	A	20051019	ZA 2005-2904	20050411
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	US 2003-618975	A	20030714		
	WO 2003-US30500	W	20030929		

OS MARPAT 140:316592

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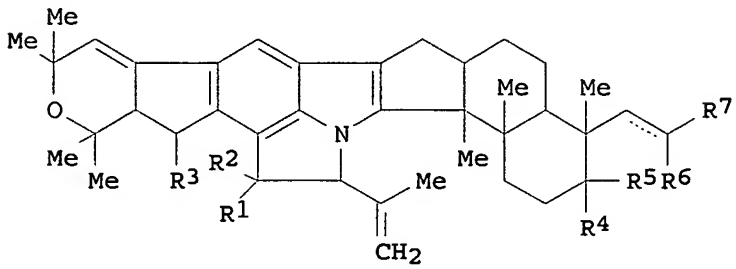

I

AB This invention provides for, inter alia, spot-on compns. for the treatment or prophylaxis of ectoparasite infestations in mammals or birds which comprise: (1) at least one nodulisporic acid derivative; (2) an acceptable liquid carrier vehicle; and (3) optionally, a crystallization inhibitor. The nodulisporic acid derivs. are I [R1 = H, (un)substituted alkyl alkenyl, alkynyl, etc.; R2,R3,R4= OH, alkoxy, OCO2H, OC(O)NH2, etc.; R1R2 = O, NOH, NNH2, etc.; R5,R6 = H; R5R6 = O; R7= CHO, CHR8CMeR9R10, etc.; R8 = H, OH, NH2, etc.; R9 = H, OH, etc.; R10 = CN, C(O)OH, CH2OH, etc.]. The preparation of tert-butylnodulisporamide and its use in a spot-on formulation to control fleas on cats, are given.

IC ICM A01N043-90
ICS A61K031-475; C07D405-06

CC 5-4 (Agrochemical Bioregulators)
Section cross-reference(s): 25

IT 205315-73-7P 315715-97-0P 315715-98-1P 315715-99-2P 315716-00-8P
315716-01-9P 315716-02-0P 387386-78-9P 412280-18-3P 470460-61-8P
470460-62-9P 470460-63-0P 678989-05-4P 678989-06-5P 678989-07-6P
678989-08-7P 678989-09-8P 678989-10-1P 678989-11-2P 678989-12-3P
678989-13-4P 678989-14-5P 678989-15-6P 678989-16-7P 678989-17-8P
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678989-88-3P 678989-89-4P 678989-90-7P 678989-91-8P 678989-92-9P
678989-93-0P 678989-94-1P 678989-95-2P 678989-96-3P 678989-97-4P
678989-98-5P 679412-17-0P 679412-18-1P
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation as spot-on ectoparasiticide)

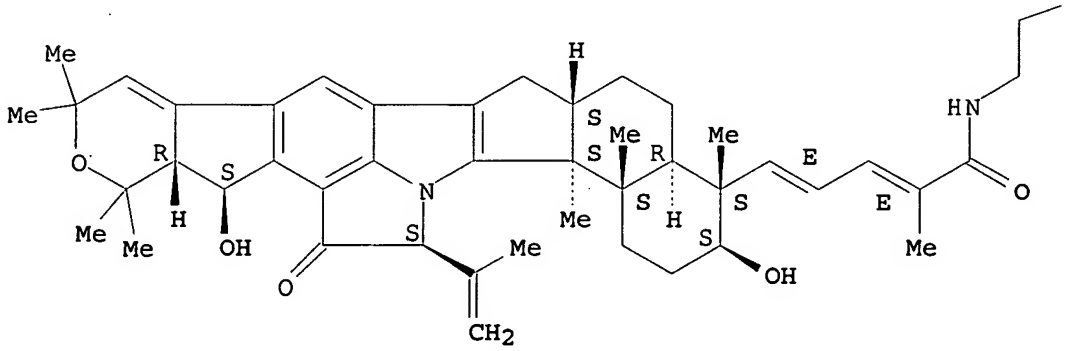
IT **678989-73-6P**
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation as spot-on ectoparasiticide)

RN 678989-73-6 HCAPLUS

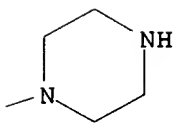
CN 2,4-Pentadienamide, 5-[(3S,4S,4aR,6aS,12aR,13S,15S,16bS,16cS)-2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13-dihydroxy-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-14-oxo-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-2-methyl-N-[2-(1-piperazinyl)ethyl]-, (2E,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



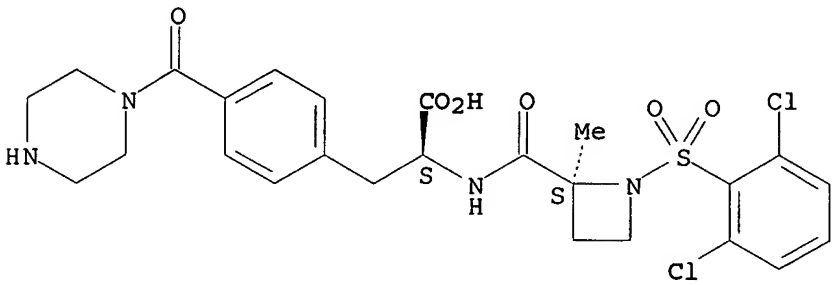
PAGE 1-B



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

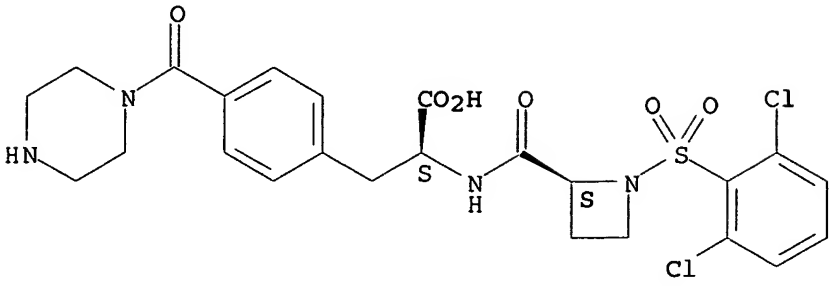
L42 ANSWER 17 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:233871 HCAPLUS
DN 141:277305
TI Synthesis of [3,5-dichlorobenzenesulfonamide-U-14C)] labeled VLA-4 antagonists
AU Yu, Nathan X.; Raab, Conrad E.; Dean, Dennis C.; Lin, Linus S.; Melillo, David G.
CS Merck Research Laboratories, RY80R-104, Department of Drug Metabolism, Rahway, NJ, 07065, USA
SO Journal of Labelled Compounds & Radiopharmaceuticals (2004), 47(2), 115-125
CODEN: JLCRD4; ISSN: 0362-4803
PB John Wiley & Sons Ltd.
DT Journal
LA English
OS CASREACT 141:277305
AB Radiolabeled tracers were required for the development of a series of VLA-4 antagonists. A method to synthesize [U-14C]3,5-dichlorobenzenesulfonyl chloride was developed. From this key intermediate, various tracers were prepared in high yield.
CC 25-13 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 74
IT **Isotope** indicators
(preparation of 14C-labeled (dichlorophenylsulfonyl)azetidinecarboxamides as radiotracers via amidation of azetidinecarboxamides with 14C-labeled dichlorophenylsulfonyl chloride followed by hydrolysis)
IT **757977-77-8P 757977-78-9P 757977-79-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of 14C-labeled (dichlorophenylsulfonyl)azetidinecarboxamides as radiotracers via amidation of azetidinecarboxamides with 14C-labeled dichlorophenylsulfonyl chloride followed by hydrolysis and deprotection)
IT **757977-77-8P 757977-78-9P 757977-79-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of 14C-labeled (dichlorophenylsulfonyl)azetidinecarboxamides as radiotracers via amidation of azetidinecarboxamides with 14C-labeled dichlorophenylsulfonyl chloride followed by hydrolysis and deprotection)
RN 757977-77-8 HCAPLUS
CN L-Phenylalanine, N-[[(2S)-1-[(2,6-dichlorophenyl)sulfonyl]-2-methyl-2-azetidinyl]carbonyl]-4-(1-piperazinylcarbonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



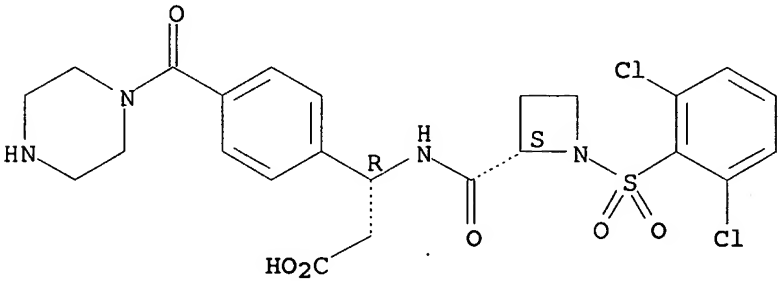
RN 757977-78-9 HCAPLUS
CN L-Phenylalanine, N-[[(2S)-1-[(2,6-dichlorophenyl)sulfonyl]-2-azetidinyl]carbonyl]-4-(1-piperazinylcarbonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 757977-79-0 HCAPLUS
CN Benzenepropanoic acid, β-[[[(2S)-1-[(2,6-dichlorophenyl)sulfonyl]-2-azetidinyl]carbonyl]amino]-4-(1-piperazinylcarbonyl)-, labeled with carbon-14, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 18 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:855935 HCAPLUS
DN 139:350742
TI Preparation of labeled oxazinocarbazoles as diagnostic agents
IN Ten Brink, Ruth Elizabeth; Merchant, Kalpana M.; McCarthy, Timothy J.
PA Pharmacia & Upjohn Company, USA
SO PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

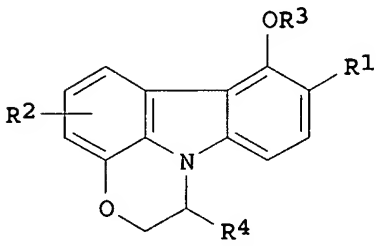
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003089438	A1	20031030	WO 2003-US8828	20030408

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

	AU 2003222038	A1	20031103	AU 2003-222038	20030408
	EP 1495031	A1	20050112	EP 2003-718022	20030408
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	US 6932961	B1	20050823	US 2003-408956	20030408
	JP 2005537226	T2	20051208	JP 2003-586158	20030408
PRAI	US 2002-372919P	P	20020416		
	WO 2003-US8828	W	20030408		

OS MARPAT 139:350742

GI



I

AB Title compds. I [R1 = H, halo; R2 = H, alkyl; R3 = (CH2)mNR5R9; R4 = aryl; aryl = Ph, naphthyl, optionally substituted with ≥1 R10; R8, R9 = H, alkyl hydroxyalkyl, CHO, provided that only 1 of R8, R9 = CHO and the other = H; R8R9N = 5-7 membered heterocyclic ring including N(Y); Y = H, alkyl; R10 = halo, OH, CN, CF3, alkyl, NH2; m = 2, 3, 4; wherein the compound includes an **isotopic** label] were prepared Thus, 7-(2-chloroethoxy)-1-phenyl-1,2-dihydro-[1,4]oxazino(2,3,4-jk)carbazole (I; R1 = R2 = H; R3 = CH2CH2Cl, R4 = Ph) (prepn given) is added sodium iodide (0.113 g, 0.751 mmol), potassium carbonate (0.207 g, 1.5 mmol), and ethanolamine (0.046 g, 0.751 mmol). The mixture is heated at 85 °C for 17 h. The temperature is then increased to 90 °C and the mixture is allowed to stir for another 5 h to give 2-[[2-[[1-Phenyl-1,2-dihydro-[1,4]oxazino(2,3,4-jk)carbazol-7-yl]oxy]ethyl]amino]-1-ethanol (I; R1 = R2 = H, R3 = CH2CH2NHCH2CH2OH, R4 = Ph) (II). II showed Ki = 1.1 nM in a 5-HT6 receptor binding assay.

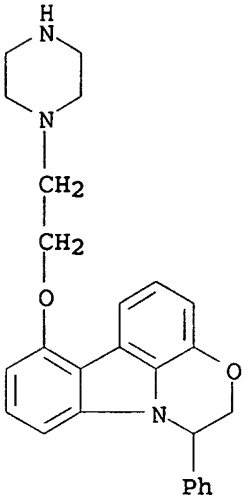
IC ICM C07D498-06
ICS C07B059-00; A61K051-04; C07M005-00

CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 9, 63

IT 324816-97-9P 324817-01-8P 324817-05-2P 324817-07-4P 324817-09-6P
324817-11-0P 324817-13-2P 324817-15-4P 324817-17-6P
324817-21-2P 324817-23-4P 324817-29-0P 324817-31-4P
324817-35-8P 324817-37-0P 324817-39-2P 324817-41-6P 324817-43-8P
324817-45-0P 324817-47-2P 324817-49-4P 324818-09-9P 324818-11-3P
324818-13-5P 618895-95-7P 618896-00-7P
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of labeled oxazinocarbazoles as diagnostic agents)

IT **324817-21-2P**
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of labeled oxazinocarbazoles as diagnostic agents)

RN 324817-21-2 HCAPLUS
CN [1,4]Oxazino[2,3,4-jk]carbazole, 1,2-dihydro-1-phenyl-7-[2-(1-piperazinyl)ethoxy]- (9CI) (CA INDEX NAME)

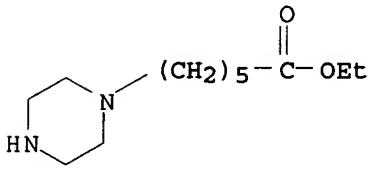


RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 19 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:837417 HCAPLUS
DN 139:335081
TI Method for characterizing peptides and proteins by MALDI using analyte labeling with light-absorbing tags
IN Thompson, Andrew Hugin; Hamon, Christian; Kuhn, Karsten; Meyer, Markus; Juergen, Schafer; Neumann, Thomas
PA Xzillion Gmbh & Co. Kg, Germany
SO PCT Int. Appl., 106 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003087839	A1	20031023	WO 2003-GB1485	20030404
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2480836	AA	20031023	CA 2003-2480836	20030404
	AU 2003224253	A1	20031027	AU 2003-224253	20030404
	EP 1490693	A1	20041229	EP 2003-720676	20030404
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2005521892	T2	20050721	JP 2003-584731	20030404

US 2006040334 A1 20060223 US 2005-510246 20050627
PRAI EP 2002-252440 A 20020404
WO 2003-GB1485 W 20030404
OS MARPAT 139:335081
AB Provided is a method for characterizing an analyte, especially peptides and proteins by matrix assisted laser desorption ionization (MALDI) mass spectrometry, which method comprises: (a) labeling the analyte with a light-absorbing label that absorbs light at a pre-determined frequency, to form a labeled analyte; (b) embedding the labeled analyte in a matrix formed from at least one compound that absorbs light, to form an embedded labeled analyte; (c) desorbing the embedded labeled analyte by exposing it to light having the pre-determined frequency, to form a desorbed analyte; and (d) detecting the desorbed analyte by mass spectrometry to characterize the analyte. The synthesis of light absorbing labels and their reaction with resin-bound peptides is presented. The invention also concerns a MALDI test kit that includes arrays of labels and a matrix.
IC ICM G01N033-68
ICS C12Q001-68; C07K001-13
CC 9-5 (Biochemical Methods)
IT **Isotopes**
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(method for characterizing peptides and proteins by MALDI using analyte labeling with light-absorbing tags)
IT 61435-75-4P 62708-58-1P 596810-54-7P 614757-16-3P 614757-18-5P
614757-19-6P 614757-35-6P 614757-36-7P 614757-37-8P 614757-38-9P
614757-39-0P 614757-40-3P 614757-41-4P 614757-42-5P
614757-43-6P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(method for characterizing peptides and proteins by MALDI using analyte labeling with light-absorbing tags)
IT **614757-39-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(method for characterizing peptides and proteins by MALDI using analyte labeling with light-absorbing tags)
RN 614757-39-0 HCAPLUS
CN 1-Piperazinehexanoic acid, ethyl ester (9CI) (CA INDEX NAME)



RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 20 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:585629 HCAPLUS
DN 139:261258
TI Safety-Catch Linker Strategies for the Production of Radiopharmaceuticals Labeled with Positron-Emitting **Isotopes**
AU Maclean, Derek; Zhu, Jiang; Chen, Mingying; Hale, Ron; Satymurthy, Nagichettiar; Barrio, Jorge R.
CS Affymax Research Institute, Palo Alto, CA, 94304, USA
SO Journal of the American Chemical Society (2003), 125(34), 10168-10169

CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 139:261258
AB A novel synthetic strategy for compds. labeled with the positron-emitting **isotope** carbon-11 is described. The use of precursors attached to a solid support via so-called safety-catch linkers allows selective release of radiolabeled material, leaving unreacted precursor attached to the support. Two different linkers demonstrate the application to the preparation of radiolabeled N-alkyl tertiary amines and N-alkylsulfonamides. This technique is expected to lead to more widespread use of positron emission tomog. for the in vivo anal. of compound behavior. Thus, ArgoGel-Wang resin-bound 4-(4-nitrophenyl)-1-piperazinepropanoic acid (ester) was prepared Product release from this was effected via methylation, thus releasing ArgoGel-Wang resin-bound 2-propenoic acid (ester) and 1-methyl-4-(4-nitrophenyl)piperazine. Quaternization of ArgoGel-Wang resin-bound 4-(4-nitrophenyl)-1-piperazinepropanoic acid (ester) with iodo-11C-methane and subsequent product release gave 1-(methyl-11C)-4-(4-nitrophenyl)piperazine. Non-methylated product was not released.
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
ST safety catch linker radiopharmaceutical label positron emitting **isotope**; combinatorial library linker radiopharmaceutical label positron emitting **isotope**; methylation safety catch linker radiopharmaceutical label positron emitting **isotope**; alkylation safety catch linker radiopharmaceutical label positron emitting **isotope**; methylpiperazine radiolabel prepn positron emitting **isotope**; cyclic amine e radiolabel prepn positron emitting **isotope**; tertiary amine radiolabel positron emitting **isotope**
IT Sulfonamides
RL: SPN (Synthetic preparation); PREP (Preparation)
(N-Me sulfonamides; safety-catch linker strategies for production of radiopharmaceuticals labeled with positron-emitting **isotopes**)
IT Amines, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclic, radiolabeled tertiary amines; safety-catch linker strategies for production of radiopharmaceuticals labeled with positron-emitting **isotopes**)
IT Alkylation
Combinatorial library
Methylation
(safety-catch linker strategies for production of radiopharmaceuticals labeled with positron-emitting **isotopes**)
IT Amines, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(tertiary, radiolabeled tertiary amines; safety-catch linker strategies for production of radiopharmaceuticals labeled with positron-emitting **isotopes**)
IT 79-10-7DP, 2-Propenoic acid, ArgoGel-Wang resin-bound
RL: PNU (Preparation, unclassified); PREP (Preparation)
(safety-catch linker strategies for production of radiopharmaceuticals labeled with positron-emitting **isotopes**)
IT 74-88-4, Iodomethane, reactions 110-73-6, 2-(Ethylamino)ethanol 110-85-0, Piperazine, reactions 110-89-4, Piperidine, reactions 111-42-2, 2,2'-Iminobis[ethanol], reactions 624-78-2, N-Methylethanamine 6269-89-2, 1-(4-Nitrophenyl)piperazine 10375-59-4, Carbon-11C dioxide 207996-54-1, ArgoGel-Wang-OH 546140-76-5, 4,6-Dichloro-N-[(4-fluorophenyl)methyl]-1,3,5-Triazin-2-amine 603111-89-3D, N'-resin-bound

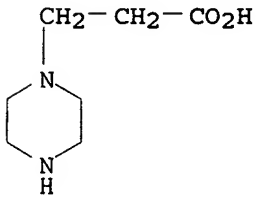
RL: RCT (Reactant); RACT (Reactant or reagent)
(safety-catch linker strategies for production of radiopharmaceuticals labeled with positron-emitting **isotopes**)

IT **27245-31-4DP**, 1-Piperazinepropanoic acid, ArgoGel-Wang resin-bound 54245-42-0P, Iodo-11C-methane 108911-74-6DP, 4-(4-Nitrophenyl)-1-piperazinepropanoic acid, ArgoGel-Wang resin-bound 164982-99-4DP, 2-Propenoic acid (4-hydroxyphenyl)methyl ester, ArgoGel-Wang resin-bound 603111-88-2DP, 4-(4-Nitrophenyl)-1-piperazinepropanoic acid (4-hydroxyphenyl)methyl ester, ArgoGel-Wang resin-bound 603111-91-7DP, N'-resin-bound 603111-96-2DP, ArgoGel-Wang resin-bound 603111-97-3DP, ArgoGel-Wang resin-bound 603111-99-5DP, ArgoGel-Wang resin-bound 603112-01-2DP, ArgoGel-Wang resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(safety-catch linker strategies for production of radiopharmaceuticals labeled with positron-emitting **isotopes**)

IT 6319-45-5P, N-Methyl-4-nitrobenzenesulfonamide 16155-03-6P, 1-Methyl-4-(4-nitrophenyl)piperazine 603111-89-3P 603111-91-7P 603111-94-0P, 1-(Methyl-11C)-4-(4-nitrophenyl)piperazine 603112-02-3P 603112-03-4P 603112-04-5P 603112-05-6P 603112-06-7P 603112-07-8P 603112-08-9P 603112-09-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(safety-catch linker strategies for production of radiopharmaceuticals labeled with positron-emitting **isotopes**)

IT **27245-31-4DP**, 1-Piperazinepropanoic acid, ArgoGel-Wang resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(safety-catch linker strategies for production of radiopharmaceuticals labeled with positron-emitting **isotopes**)

RN 27245-31-4 HCAPLUS
CN 1-Piperazinepropanoic acid (9CI) (CA INDEX NAME)



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 21 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:376987 HCAPLUS
DN 138:385215
TI Preparation of **isotopically**-coded affinity markers for mass spectrometric analysis of proteins
IN Lerchen, Hans-Georg; Siegmund, Hans-Ulrich; Immler, Dorian; Schumacher, Andreas; Auriel, Daniel
PA Bayer Aktiengesellschaft, Germany
SO PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI WO 2003040288 A2 20030515 WO 2002-EP12105 20021030
WO 2003040288 A3 20031211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
DE 10234415 A1 20030522 DE 2002-10234415 20020729
CA 2466328 AA 20030515 CA 2002-2466328 20021030
EP 1446665 A2 20040818 EP 2002-774759 20021030
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
EP 1477493 A1 20041117 EP 2003-9894 20030515
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
US 2005049406 A1 20050303 US 2004-494999 20041029
PRAI DE 2001-10154745 A 20011109
DE 2002-10234415 A 20020729
WO 2002-EP12105 W 20021030
OS MARPAT 138:385215
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention concerns **isotopically**-coded affinity markers (ICAT), A-L-PRG, e.g., I [A = affinity ligand (especially biotin); PRG = protein reactive group (maleimido, chloroalkyl, acryloyl); L = linker, L*; Z = NHCH2CO; L' = bridge between piperazines; R, R' = piperazine ring, D-, L- or (±)-amino acid; Z' = COCH2NH; k, l, m, n = 0 - 10, whereby k + l + m + n = 1 - 40] or its salts, for mass spectrometric anal. of proteins, and the preparation and use of said markers. Thus, biotin derivative I was prepared from piperazide II via regioselective deprotection, N-acylation with 3-maleimidopropionic acid, N-deprotection and coupling of, with biotin derivative III. Mass spectrometric anal. of proteins was carried out using ICAT I.

IC ICM C12N
CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 9, 34
ST **isotopically** coded affinity marker prepn protein mass spectral analysis
IT Affinity labeling
(**isotopically**-coded markers; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)
IT Mass spectrometry
(preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)
IT Peptides, analysis
Proteins
RL: ANT (Analyte); ANST (Analytical study)
(preparation of **isotopically**-coded affinity markers for mass

spectrometric anal. of proteins)

IT 173690-53-4, [4-(Fmoc-amino)phenyl]acetic acid 185116-43-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-acylation by, of NovaSyn TG resin; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 67836-01-5, [1,2-13C2]-Glycine
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-protection of; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 211057-02-2P, [1,2-13C2,15N]-Glycine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(N-protection of; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 205688-13-7, N-(Fmoc)-p-phenylenediamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, biotin acid chloride; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 166410-32-8, N-(Fmoc)-1,2-ethylenediamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of 4-aminobenzoic acid; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 57260-71-6, N-Boc-piperazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of Fmoc-glycine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 4403-71-8, 4-Aminobenzyl amine
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of biotin; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 110-85-0, Piperazine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of glycine derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 219312-89-7, N-Fmoc-piperazine 373608-48-1, N-(3-Aminopropyl)-N'-(tert-butoxycarbonyl)piperazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of oxalyl chloride; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 29022-11-5, Fmoc-glycine
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, by Boc-piperazine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 7423-55-4, 3-Maleimidopropionic acid 55750-53-3, ε-Maleimidohexanoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, by biotin piperazide derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 150-13-0, 4-Aminobenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, by mono(Fmoc)ethylenediamine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 4530-20-5, Boc-glycine 55750-61-3, Maleimidoacetic acid N-hydroxysuccinimidyl ester 242459-97-8, N-(2-Carboxyethyl)-N'-(tert-butoxycarbonyl)piperazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, by piperazine derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 2899-60-7, N-(Benzyloxycarbonyl)glycine N-hydroxysuccinimidyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, by piperazine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 79-04-9, Chloroacetyl chloride 814-68-6, Acryloyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, with biotin piperazide derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 58-85-5, Biotin
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525586-61-2P
RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and HCl salt formation of; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-48-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and N-acylation of, with maleimidobutyric acid; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525583-79-3P 525587-33-1P 525587-35-3P, N-Boc-[1,2-13C2]-Glycine methyl ester 525587-39-7P 525587-45-5P 525587-46-6P 525587-49-9P
525587-52-4P 525587-54-6P 525587-55-7P 525587-56-8P 525587-58-0P
525587-60-4P 525587-62-6P 525587-64-8P 525587-66-0P 525587-68-2P
525587-70-6P 525587-72-8P 525587-74-0P 525587-80-8P 525587-82-0P
525587-84-2P 525587-86-4P 525587-89-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and N-deprotection of; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT **525587-93-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and amidation by, of Boc-glycine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-92-2P, N-Cbz-Glycine-1,2-13C,15N
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with Glycine-1,2-13C Me ester; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-36-4P, [1,2-13C2]-Glycine methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with N-Boc-[1,2-13C2]-Glycine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-57-9P 525587-59-1P 525587-61-5P 525587-63-7P 525587-65-9P
525587-67-1P 525587-69-3P 525587-71-7P 525587-73-9P 525587-83-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with biotin derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-85-3P 525587-87-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with maleimidobutyric acid; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 145142-99-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification or coupling of, with Glycine-1,2-13C Me ester; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-47-7P 525587-76-2P 525587-78-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolytic N-deprotection of; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-91-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. cyclization of; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525586-94-1P, [2,3,5,6-13C4-1,4-15N]-Piperazine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and partial N-protection of; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT **525587-94-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with Bis(Boc)histidine ester; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT **525587-43-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with Boc-glycine-N-carboxylic anhydride; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-77-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with Cbz-leucine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT **525587-40-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with Fmoc-glycine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT **105807-56-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with N-(Boc-glycyl)glycine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 352359-09-2P **525586-96-3P 525586-98-5P**,
N-Fmoc-[2,3,5,6-13C4-1,4-15N]-Piperazine 525586-99-6P

525587-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with N-oxalylpiperazine derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-75-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with NovaSyn TG resin isothiocyanate derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT **525586-90-7P** 525586-92-9P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with amino acid or N-oxalylpiperazine derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-88-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with aminopropylated silica gel thiocyanate derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT **525587-21-7P 525587-22-8P 525587-23-9P**
525587-28-4P 525587-30-8P 525587-32-0P
525587-51-3P 525587-81-9P 525587-95-5P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with biotin derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525583-46-4P 525583-47-5P 525583-48-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with linker compds.; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-20-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with maleimidoalkanoic acids; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-79-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with maleimidobutyric acid; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-53-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with maleimidopropionic acid; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 160624-42-0P 525583-78-2P 525583-81-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with thiophosgene; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-37-5P, 2,5-Piperazinedione-2,3,5,6-13C4
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of, with borane-THF complex; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-03-5P 525587-18-2P 525587-24-0P 525587-25-1P 525587-26-2P
525587-34-2P 525587-44-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and regioselective N-deprotection of; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 71160-41-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and regioselective reaction of, with biotin derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-38-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and saponification of; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525586-41-8P 525586-42-9P 525586-43-0P 525586-44-1P 525586-45-2P
525586-46-3P 525586-47-4P 525586-48-5P 525586-49-6P 525586-50-9P
525586-51-0P 525586-52-1P 525586-53-2P 525586-54-3P 525586-55-4P
525586-56-5P 525586-57-6P 525586-58-7P 525586-59-8P 525586-60-1P
525586-62-3P 525586-63-4P 525586-64-5P 525586-65-6P 525586-66-7P
525586-67-8P 525586-68-9P 525586-69-0P 525586-70-3P 525586-71-4P
525586-72-5P 525586-73-6P 525586-74-7P 525586-75-8P 525586-76-9P
525586-77-0P 525586-78-1P 525586-79-2P 525586-80-5P 525586-81-6P
525586-82-7DP, NovaSyn TG resin-bound amide 525586-83-8P 525586-84-9P
525586-85-0P 525586-86-1P 525586-87-2P 525586-88-3DP,
aminopropylated silica gel-bound amide
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT **525586-97-4P**, N-Boc-[2,3,5,6-13C4-1,4-15N]-Piperazine
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525586-93-0P, [2,3,5,6-13C4]-Piperazine
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-41-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, carbonylation and reaction of, with piperazine derivative; preparation

of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-42-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, regioselective N-deprotection and reaction of, with N-(Boc-glycyl)glycine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-01-3P 525587-02-4P 525587-04-6P 525587-05-7P 525587-06-8P
525587-07-9P 525587-08-0P 525587-09-1P 525587-10-4P 525587-11-5P
525587-12-6P 525587-13-7P 525587-14-8P 525587-15-9P 525587-16-0P
525587-17-1P 525587-19-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, regioselective N-deprotection and reaction of, with biotin derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 2018-66-8, Cbz-L-leucine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with N-leucylglutamine piperazide derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 4666-16-4, N-Cbz-L-glutamic acid γ-(tert butyl) α-(N-hydroxysuccinimidyl) diester
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with glutamine piperazide derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 57078-98-5P, ω-Maleimidobutyric acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction of, with oxalyl di(piperazide) derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 2566-19-0, N-(N-Cbz-glycyl)glycine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with oxalyl dipiperazide derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 31972-52-8, N-(N-Boc-glycyl)glycine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with oxalyldipiperazide; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 88743-98-0, N-(N-Fmoc-L-leucyl)-L-leucine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with piperazide derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

IT 1676-90-0, N-Boc-L-asparaginic acid γ-(tert-butyl) ester
3303-84-2, Boc-β-alanine 3392-10-7, N-Boc-L-proline N-hydroxysuccinimidyl ester 7536-55-2, N-Boc-L-asparagine 13726-84-6, N-Boc-L-glutamic acid γ-(tert-butyl) ester 13734-41-3, N-Boc-L-valine 22838-58-0, N-Boc-D-valine 25616-02-8, Bis(Boc)-L-histidine N-hydroxysuccinimidyl ester 142955-50-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with piperazine derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

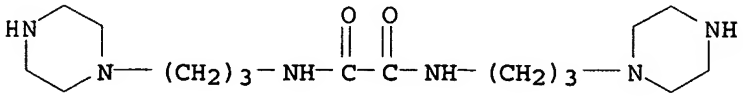
IT 7631-86-9D, Silicon dioxide, aminopropylated 210106-36-8, NovaSyn TG
RL: RCT (Reactant); RACT (Reactant or reagent)
(support for **isotopically**-coded affinity markers; preparation of **isotopically**-coded affinity markers for mass spectrometric

anal. of proteins)

IT **525587-93-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and amidation by, of Boc-glycine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

RN 525587-93-3 HCAPLUS

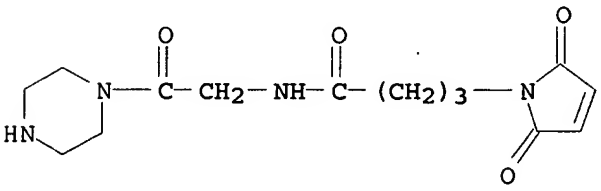
CN Ethanediamide, N,N'-bis[3-(1-piperazinyl)propyl]- (9CI) (CA INDEX NAME)



IT **525587-94-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with Bis(Boc)histidine ester; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

RN 525587-94-4 HCAPLUS

CN 1H-Pyrrole-1-butanamide, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-(1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)

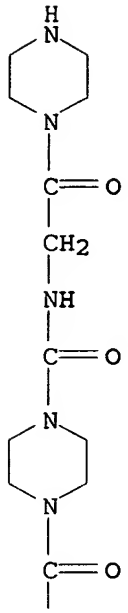


IT **525587-43-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with Boc-glycine-N-carboxylic anhydride; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

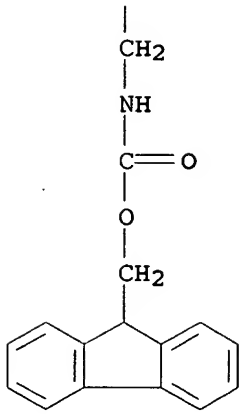
RN 525587-43-3 HCAPLUS

CN Carbamic acid, [2-oxo-2-[4-[[[2-oxo-2-(1-piperazinyl)ethyl]amino]carbonyl]-1-piperazinyl]ethyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



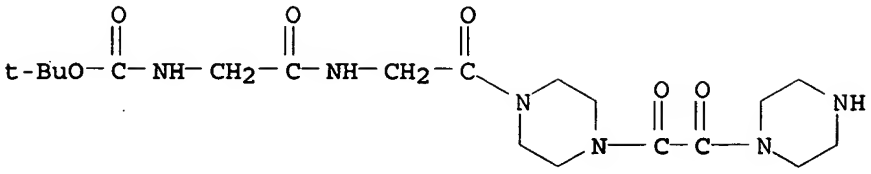
PAGE 2-A



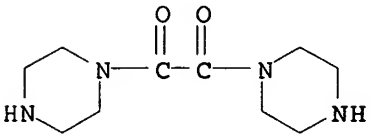
IT **525587-40-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with Fmoc-glycine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)

RN 525587-40-0 HCAPLUS

CN Carbamic acid, [2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinylacetyl)-1-piperazinyl]ethyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



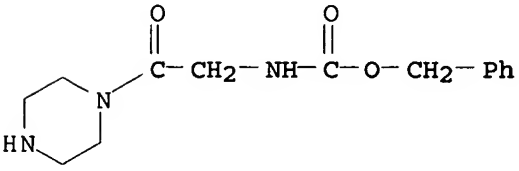
IT **105807-56-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with N-(Boc-glycyl)glycine; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)
RN 105807-56-5 HCAPLUS
CN Piperazine, 1,1'-(1,2-dioxo-1,2-ethanediyl)bis- (9CI) (CA INDEX NAME)



IT **525586-96-3P 525586-98-5P**, N-Fmoc-[2,3,5,6-13C4-1,4-15N]-Piperazine **525587-00-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with N-oxalylpiperazine derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)
RN 525586-96-3 HCAPLUS
CN Carbamic acid, [2-oxo-2-(1-piperazinyl)ethyl]-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

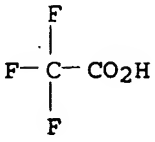
CM 1

CRN 525586-95-2
CMF C14 H19 N3 O3

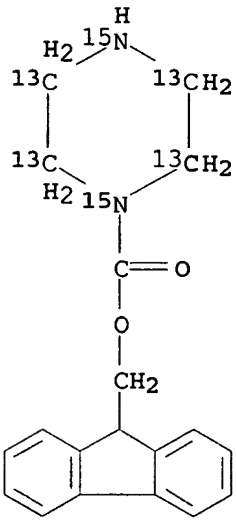


CM 2

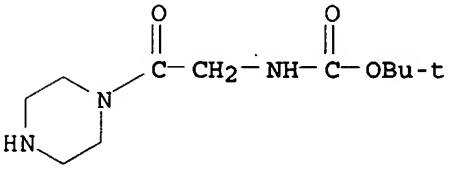
CRN 76-05-1
CMF C2 H F3 O2



RN 525586-98-5 HCAPLUS
CN 1-Piperazine-2,3,5,6-13C4-1,4-15N2-carboxylic acid, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)



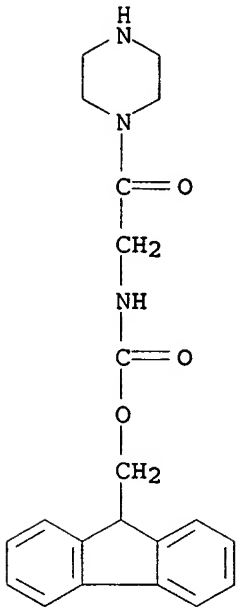
RN 525587-00-2 HCAPLUS
CN Carbamic acid, [2-oxo-2-(1-piperazinyl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



IT **525586-90-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with amino acid or N-oxalylpiperazine derivative;
preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)
RN 525586-90-7 HCAPLUS
CN Carbamic acid, [2-oxo-2-(1-piperazinyl)ethyl]-, 9H-fluoren-9-ylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

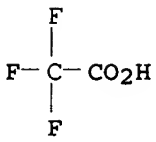
CM 1

CRN 525586-89-4
CMF C21 H23 N3 O3



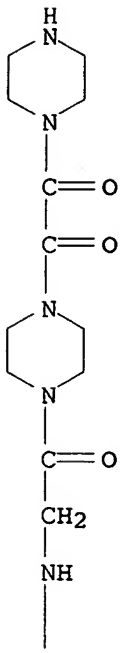
CM 2

CRN 76-05-1
CMF C2 H F3 O2

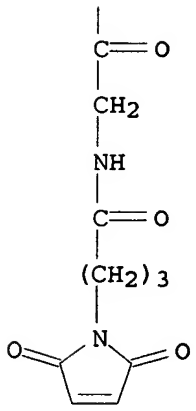


IT **525587-21-7P 525587-22-8P 525587-23-9P**
525587-28-4P 525587-30-8P 525587-32-0P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with biotin derivative; preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)
RN 525587-21-7 HCAPLUS
CN 1H-Pyrrole-1-butanamide, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinylacetyl)-1-piperazinyl]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

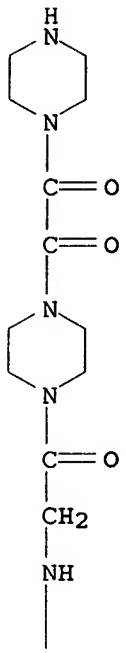


PAGE 2-A

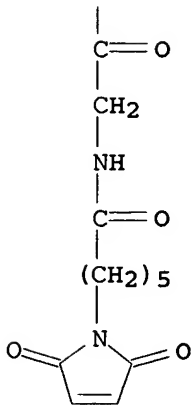


RN 525587-22-8 HCAPLUS
CN 1H-Pyrrole-1-hexanamide, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinylacetyl)-1-piperazinyl]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

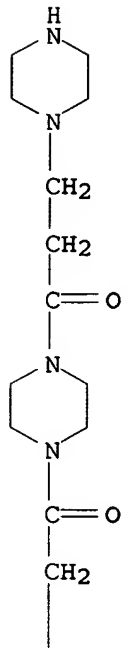


PAGE 2-A

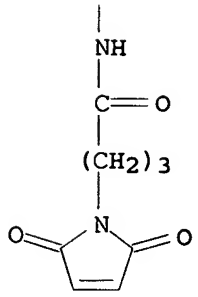


RN 525587-23-9 HCAPLUS
CN 1H-Pyrrole-1-butanamide, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[4-[1-oxo-3-(1-piperazinyl)propyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

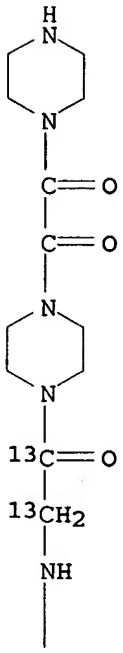


RN 525587-28-4 HCAPLUS
CN 1H-Pyrrole-1-butanamide-15N, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinylacetyl)-1-piperazinyl]ethyl-13C2]amino]ethyl-13C2]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

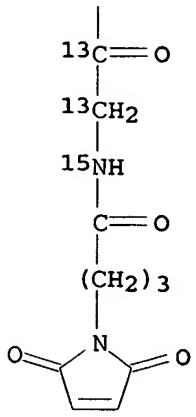
CM 1

CRN 525587-27-3
CMF C22 H31 N7 O7

PAGE 1-A

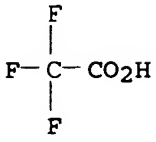


PAGE 2-A



CM 2

CRN 76-05-1
CMF C2 H F3 O2

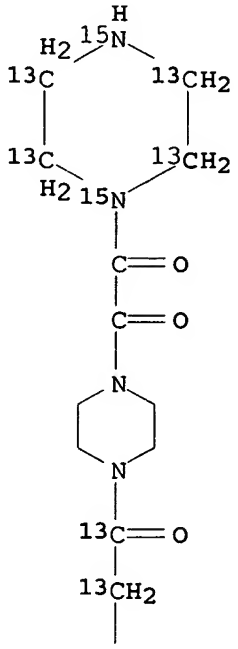


RN 525587-30-8 HCAPLUS
CN 1H-Pyrrole-1-butanamide-15N, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinyl-2,3,5,6-13C4-1,4-15N2-acetyl)-1-piperazinyl]ethyl-13C2]amino]ethyl-13C2]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

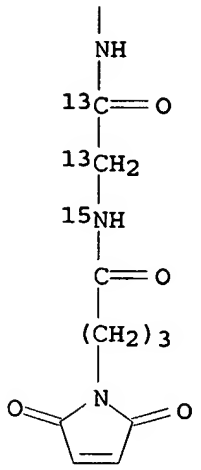
CM 1

CRN 525587-29-5
CMF C22 H31 N7 O7

PAGE 1-A

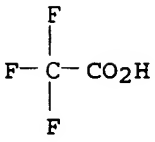


PAGE 2-A



CM 2

CRN 76-05-1
CMF C2 H F3 O2

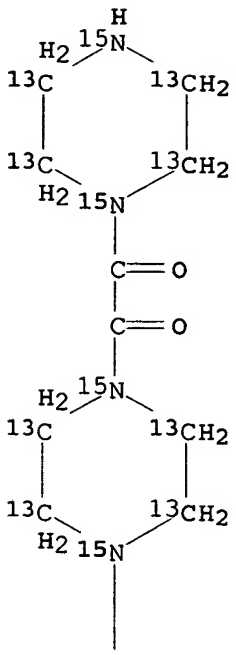


RN 525587-32-0 HCAPLUS
CN 1H-Pyrrole-1-butanamide-15N, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinyl-2,3,5,6-13C4-1,4-15N2-acetyl)-1-piperazinyl-2,3,5,6-13C4-1,4-15N2-]ethyl-13C2]amino]ethyl-13C2]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

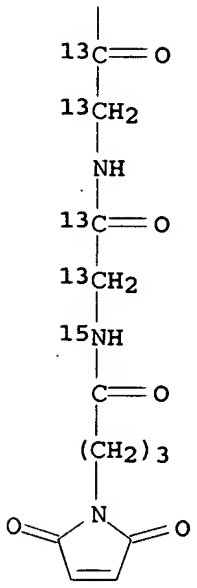
CM 1

CRN 525587-31-9
CMF C22 H31 N7 O7

PAGE 1-A

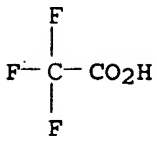


PAGE 2-A

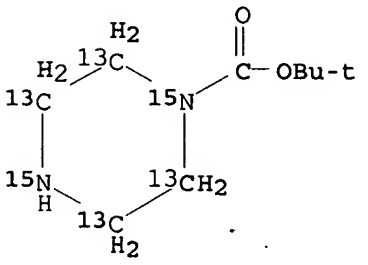


CM 2

CRN 76-05-1
CMF C2 H F3 O2



IT **525586-97-4P**, N-Boc-[2,3,5,6-13C4-1,4-15N]-Piperazine
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of **isotopically**-coded affinity markers for mass spectrometric anal. of proteins)
RN 525586-97-4 HCAPLUS
CN 1-Piperazine-2,3,5,6-13C4-1,4-15N2-carboxylic acid, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

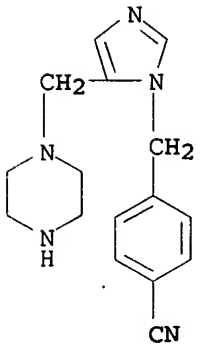


L42 ANSWER 22 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2002:450255 HCAPLUS
DN 137:17431
TI Geranylgeranyl transferase inhibitor screening assay
IN Eng, Wai-si; Lobell, Robert B.; Lumma, William C.; Smith, Anthony M.
PA USA
SO U.S. Pat. Appl. Publ., 42 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

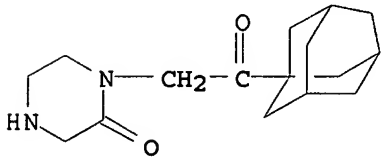
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2002072081	A1	20020613	US 2001-947903	20010906
PRAI US 2000-230270P	P	20000906		

OS MARPAT 137:17431
AB The invention concerns a GGTase-I competitive binding assay which can be used to determine the relative GGTase-I inhibitory potency of test compds. The present invention is also directed toward radiolabeled geranylgeranyl-protein transferase type-I inhibitor compds. which are useful to label GGTase-I in assays, whether cell-based, tissue-based or in whole animal.
IC ICM C12Q001-48
ICS C07D043-14; C07D043-02
INCL 435015000
CC 9-8 (Biochemical Methods)
Section cross-reference(s): 1, 7
IT **Isotope** indicators
(as labels; geranylgeranyl transferase inhibitor screening assay)

IT **290819-56-6P** 291751-10-5P
RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(geranylgeranyl transferase inhibitor screening assay)
IT 10406-25-4P 183500-36-9P 252882-62-5P 291751-24-1P
291751-25-2P 434333-13-8P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(geranylgeranyl transferase inhibitor screening assay)
IT **290819-56-6P**
RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(geranylgeranyl transferase inhibitor screening assay)
RN 290819-56-6 HCAPLUS
CN Benzonitrile, 4-[[5-(1-piperazinylmethyl)-1H-imidazol-1-yl]methyl]- (9CI) (CA INDEX NAME)



IT **291751-25-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(geranylgeranyl transferase inhibitor screening assay)
RN 291751-25-2 HCAPLUS
CN Piperazinone, 1-(2-oxo-2-tricyclo[3.3.1.13,7]dec-1-ylethyl)- (9CI) (CA INDEX NAME)



L42 ANSWER 23 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2001:31737 HCAPLUS
DN 134:97533
TI Detection using dendrimers bearing labels and probes
IN Lohse, Jesper
PA Dako A/S, Den.
SO PCT Int. Appl., 131 pp.
CODEN: PIXXD2

DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001002861	A1	20010111	WO 2000-DK351	20000629
	W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2376619	AA	20010111	CA 2000-2376619	20000629
	EP 1192465	A1	20020403	EP 2000-940224	20000629
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2003503591	T2	20030128	JP 2001-508057	20000629
	US 2003077635	A1	20030424	US 2002-238732	20020911
PRAI	DK 1999-934	A	19990629		
	US 2000-606315	B1	20000629		
	WO 2000-DK351	W	20000629		

AB Novel dendrimers as well as novel dendrimer complexes are disclosed. Such dendrimers and/or dendrimer complexes may be used for the detection of various components of a sample and as detection systems and signal enhancement/amplification systems. The dendrimers and dendrimer complexes may also be used for labeling various entities/compds. Furthermore, labeling kits and detection kits comprising one or more labeled dendrimers or one or more dendrimer complexes are also one of the possible uses.

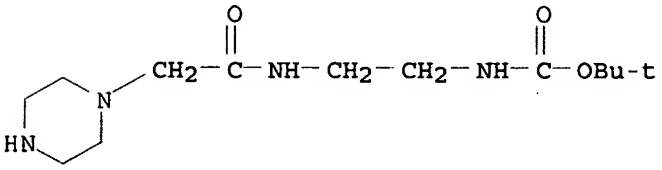
IC ICM G01N033-58
ICS C12Q001-68; C08G083-00
CC 9-16 (Biochemical Methods)
Section cross-reference(s): 3
IT Alkyl groups
Animal tissue
Blood analysis
Bond
Bone marrow
Cell
Chemiluminescent substances
Chromosome
DNA sequences
Diagnosis
Dyes
Epitopes
Fluorescent substances
Functional groups
Isotope indicators
Labels
Organ, animal
Protective groups
RNA sequences
Spin labels
Test kits
(detection using dendrimers bearing labels and probes)
IT 58-85-5DP, Biotin, reaction with dendritic polymers 144-55-8P, Carbonic acid monosodium salt, preparation 2321-07-5DP, Fluorescein, reaction with dendritic polymers 34901-14-9P 99616-36-1P 194920-62-2P

252940-86-6DP, reaction with dendritic polymers 319460-01-0P
319460-02-1P 319460-03-2P 319460-04-3P 319460-05-4P 319460-06-5P
319460-07-6P 319460-08-7P 319460-09-8P 319460-10-1P 319460-11-2P
319460-12-3P 319460-13-4P 319460-14-5P 319460-15-6P 319460-16-7P
319460-17-8P 319460-18-9P 319460-19-0P 319460-20-3P 319460-21-4P
319460-22-5P 319460-23-6P 319460-24-7P **319460-25-8P**
319460-27-0P 319460-28-1P 319460-29-2P 319932-73-5DP, reaction with dendritic polymers 319932-74-6DP, reaction with dendritic polymers
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(detection using dendrimers bearing labels and probes)

IT **319460-25-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(detection using dendrimers bearing labels and probes)

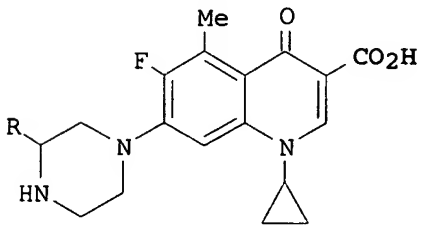
RN 319460-25-8 HCAPLUS

CN Carbamic acid, [2-[(1-piperazinylacetyl)amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 24 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:550059 HCAPLUS
DN 133:309769
TI Synthesis of stable **isotopically** labelled antibacterial agent grepafloxacin
AU Wells, Guy N.; Carr, Richard M.; Sutherland, Derek R.
CS Development Chemistry Department, Chemical Development Division, Glaxo Wellcome Medicines Research Centre, Stevenage, SG1 2NY, UK
SO Synthesis and Applications of Isotopically Labelled Compounds 1997, Proceedings of the International Symposium, 6th, Philadelphia, PA, United States, Sept. 14-18, 1997 (1998), Meeting Date 1997, 517-520. Editor(s): Heys, J. Richard; Melillo, David G. Publisher: John Wiley & Sons Ltd., Chichester, UK.
CODEN: 69AGFQ
DT Conference
LA English
GI



I

AB A symposium report on the synthesis of a stable **isotopically** labeled version, e.g. I [R = C(3H)3], of antibacterial agent grepafloxacin (I; R = Me). Anti-infectives are currently the largest category of ethical pharmaceutical products, with the majority being described for the treatment of respiratory infections. I (R = Me), licensed by Glaxo Wellcome from Otsuka, is a new generation quinolone antibiotic for the treatment of respiratory infections. I (R = Me) shows enhanced antibacterial activity against both gram-pos. and gram-neg. bacteria and has the potential to overcome micro-organism resistance to existing treatments. A stable **isotopically** labeled (SIL) version of I (R = Me) was required, as an internal standard, for the development of a high throughput mass spectrometric assay to support a bioequivalence study.

CC 26-6 (Biomolecules and Their Synthetic Analogs)

ST mass spectra std **isotopically** labeled grepafloxacin synthesis; bioequivalence **isotopically** labeled std grepafloxacin synthesis

IT Antibiotics
(quinolone, stable **isotopically**-labeled; synthesis of a stable **isotopically** labeled antibacterial agent grepafloxacin as a mass spectra internal standard)

IT Drug bioequivalence
(stable **isotopically**-labeled standard; synthesis of a stable **isotopically** labeled antibacterial agent grepafloxacin as a mass spectra internal standard)

IT Standard substances, analytical
(stable **isotopically**-labeled; synthesis of a stable **isotopically** labeled antibacterial agent grepafloxacin as a mass spectra internal standard)

IT 119914-60-2DP, Grepafloxacin, **isotopically** labeled
301673-11-0P
RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(synthesis of a stable **isotopically** labeled antibacterial agent grepafloxacin as a mass spectra internal standard)

IT 106-57-0, Piperazine-2,5-dione 109-07-9, 2-Methylpiperazine 6436-90-4, Ethyl N-benzylglycinate 7764-95-6, N-(tert-Butoxycarbonyl)-D-alanine
119916-33-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of a stable **isotopically** labeled antibacterial agent grepafloxacin as a mass spectra internal standard)

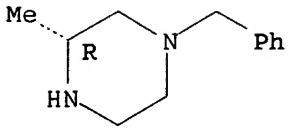
IT 42492-87-5P, 1,4-Dibenzylpiperazine-2,5-dione 75336-86-6P, (R)-2-Methylpiperazine 132871-09-1P, (R)-1-Benzyl-3-methylpiperazine-2,5-dione **132871-11-5P**, (R)-1-Benzyl-3-methylpiperazine
147578-65-2P 301673-04-1P 301673-06-3P 301673-08-5P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis of a stable **isotopically** labeled antibacterial agent grepafloxacin as a mass spectra internal standard)

IT **132871-11-5P**, (R)-1-Benzyl-3-methylpiperazine
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis of a stable **isotopically** labeled antibacterial agent grepafloxacin as a mass spectra internal standard)

RN 132871-11-5 HCAPLUS

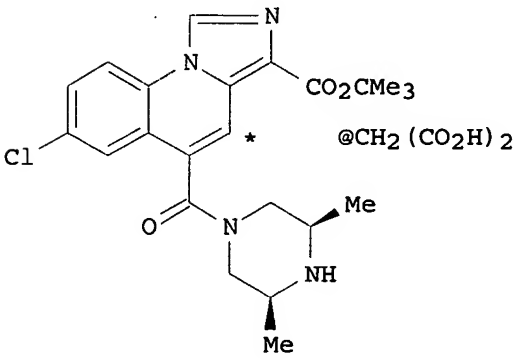
CN Piperazine, 3-methyl-1-(phenylmethyl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 25 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:550028 HCAPLUS
DN 134:162994
TI Synthesis of carbon-13 and carbon-14 **isotopically** labeled PNU-101017E, a GABAA receptor partial agonist, under development for the treatment of anxiety
AU Stolle, W. T.; Hsi, R. S. P.
CS Drug Metabolism Research, Pharmacia and Upjohn, Kalamazoo, MI, USA
SO Synthesis and Applications of Isotopically Labelled Compounds 1997, Proceedings of the International Symposium, 6th, Philadelphia, PA, United States, Sept. 14-18, 1997 (1998), Meeting Date 1997, 383-386. Editor(s): Heys, J. Richard; Melillo, David G. Publisher: John Wiley & Sons Ltd., Chichester, UK.
CODEN: 69AGFQ
DT Conference
LA English
GI



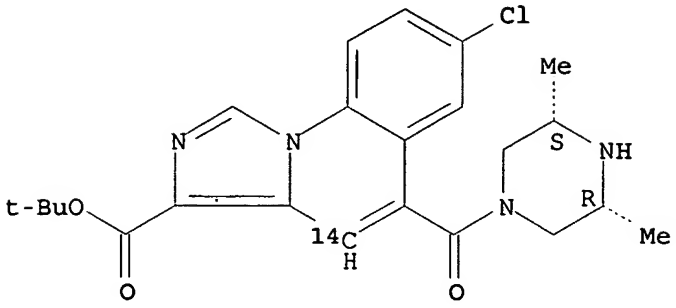
I

AB A symposium report on the preparation of PNU-101017E (I) labeled with carbon-13 or carbon-14.
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **324527-60-8P 324527-62-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
IT **324527-60-8P 324527-62-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 324527-60-8 HCAPLUS
CN Propanedioic acid, compd. with rel-1,1-dimethylethyl 7-chloro-5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]carbonyl]imidazo[1,5-a]quinoline-4-14C-3-carboxylate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 324527-59-5
CMF C23 H27 Cl N4 O3

Relative stereochemistry.



CM 2

CRN 141-82-2
CMF C3 H4 O4

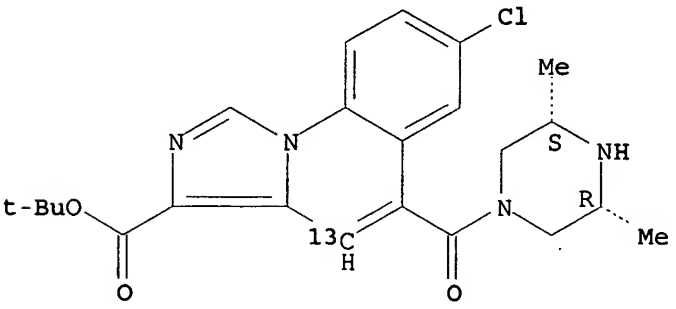
$HO_2C-CH_2-CO_2H$

RN 324527-62-0 HCAPLUS
CN Propanedioic acid, compd. with rel-1,1-dimethylethyl 7-chloro-5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]carbonyl]imidazo[1,5-a]quinoline-4-13C-3-carboxylate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 324527-61-9
CMF C23 H27 Cl N4 O3

Relative stereochemistry.



CM 2

CRN 141-82-2
CMF C3 H4 O4

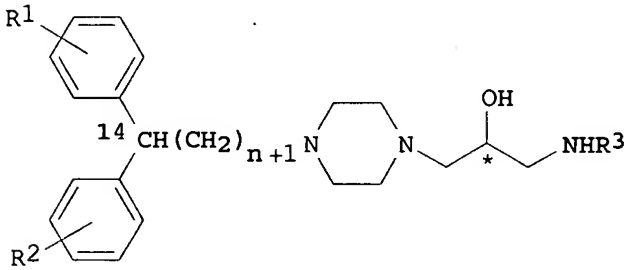
$HO_2C-CH_2-CO_2H$

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 26 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1999:188996 HCAPLUS
DN 130:252375
TI Preparation of 14C-radioactive labeled compounds, 1-(14C-diphenylalkyl)-4-(3-amino-2-hydroxypropyl)piperazine derivatives
IN Namiki, Takayuki; Yanagi, Masayuki; Kimura, Makoto; Kawakatsu, Tsuneyuki; Yamada, Koji
PA Pola Chemical Industries, Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 11071362	A2	19990316	JP 1998-192400	19980623
PRAI JP 1997-183030	A	19970624		

OS MARPAT 130:252375
GI



I

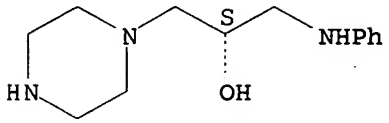
AB The title compds. [I; R1, R2 = H, halo; R3 = (un)substituted aromatic group; n = an integer of 1-5; * represents an asym. C atom], which are useful for studying drug behaviors of diphenylalkyl compds. (no data), are prepared Thus, (S)-1-(2-hydroxy-3-phenylaminopropyl)piperazine trihydrochloride 372, pulverized KI 186, K2CO3 644 mg, and 20 mL dry EtOH were sequentially added to [4-C14]4,4-bis(4-fluorophenyl)butyl bromide (282 MBq) and the resulting mixture was refluxed with stirring for 9 h to give 166 MBq of the title compound (S)-I (R1 = R2 = 4-F, n = 2, R3 = Ph) of 98.0% radiochem. purity.
IC ICM C07D295-12
ICS A61K049-00; C07C022-04; C07C025-18; C07C025-24; C07C033-34; C07C033-50; A61K051-00; C07M005-00; C07M007-00
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 6
IT Drug metabolism
Isotope indicators
(preparation of 14C-radioactive labeled N-(14C-diphenylalkyl)-N'-(aminohydroxypropyl)piperazine derivs. for studying drug behaviors)

IT 57668-61-8P, 4,4-Bis(4-fluorophenyl)butyl bromide 59455-11-7P
219994-03-3P **219994-04-4P** 219994-05-5P **219994-06-6P**
221565-22-6P 221565-23-7P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of 14C-radioactive labeled N-(14C-diphenylalkyl)-N'-(aminohydroxypropyl)piperazine derivs. for studying drug behaviors)

IT **219994-04-4P 219994-06-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of 14C-radioactive labeled N-(14C-diphenylalkyl)-N'-(aminohydroxypropyl)piperazine derivs. for studying drug behaviors)

RN 219994-04-4 HCAPLUS
CN 1-Piperazineethanol, α-[(phenylamino)methyl]-, trihydrochloride, (αS)- (9CI) (CA INDEX NAME)

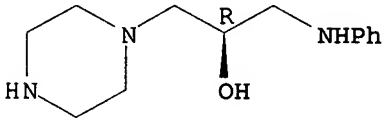
Absolute stereochemistry.



●3 HCl

RN 219994-06-6 HCAPLUS
CN 1-Piperazineethanol, α-[(phenylamino)methyl]-, trihydrochloride, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●3 HCl

L42 ANSWER 27 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:293374 HCAPLUS
DN 129:587
TI Anti-neurogenic inflammatory compounds and compositions and methods of use thereof
IN Jacobs, Robert S.; Pomponi, Shirley; Gunasekera, Sarath; Wright, Amy
PA Harbor Branch Oceanographic Institution, Inc., USA; Regents of the University of California
SO PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9818466	A2	19980507	WO 1997-US20300	19971031
	W: CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2268399	AA	19980507	CA 1997-2268399	19971031
	EP 935463	A2	19990818	EP 1997-946578	19971031
	EP 935463	B1	20040121		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	US 5955462	A	19990921	US 1997-961475	19971031
	JP 2001503414	T2	20010313	JP 1998-520828	19971031
	AT 258050	E	20040215	AT 1997-946578	19971031
	ES 2212814	T3	20040801	ES 1997-946578	19971031
	US 6090811	A	20000718	US 1999-356282	19990716
PRAI	US 1996-30261P	P	19961031		
	US 1997-961475	A1	19971031		
	WO 1997-US20300	W	19971031		

OS MARPAT 129:587

AB A novel use for the class of biol. active bis-heterocyclic, e.g., bis-indole alkaloid compds., which have been named topsentins, bromotopsentins, homocarbonyltopsentins, nortopsentins, hamacanthins, bis-indole ethylamines, or dragmacidins, pharmaceutical compns. containing the compds., methods of producing the compds., and methods of using the compds. are disclosed. Specifically, the novel utility pertains to the anti-neurogenic inflammatory properties exhibited by the bis-indole compds. and their analogs. The preparation of these compds. is described and pharmacol. data are given.

IC ICM A61K031-40
ICS A61K031-415; A61K031-495

CC 1-7 (Pharmacology)
Section cross-reference(s): 31, 63

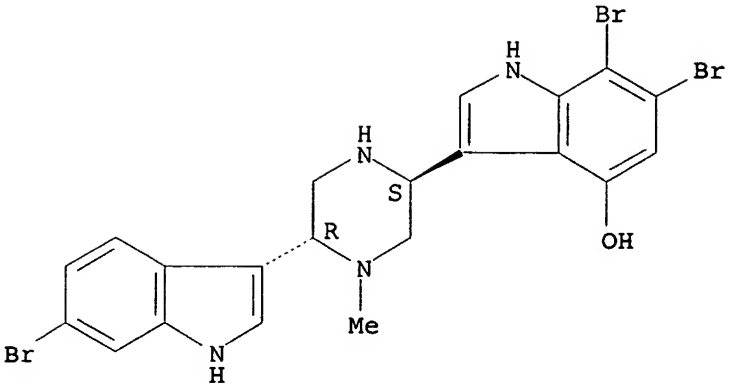
IT 112515-42-1P, Deoxytopsentin 112515-43-2P, Topsentin 112515-44-3P, Bromotopsentin **114582-72-8P**, Dragmacidin 116725-88-3P, **Isotopsentin** 116725-89-4P, Hydroxytopsentin 116725-90-7P, Neotopsentin 116725-91-8P, Neoisotopsentin 116747-41-2P, Neohydroxytopsentin 134029-43-9P, Nortopsentin A 134029-44-0P, Nortopsentin B 134029-45-1P, Nortopsentin C 135077-20-2P 142979-34-8P, Dragmacidin d 154269-22-4P 160098-92-0P, Hamacanthine A 160098-93-1P, Hamacanthine B 172286-77-0P 172286-78-1P 207445-50-9P 207445-51-0P 207445-55-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(anti-neurogenic inflammatory compds.)

IT **114582-72-8P**, Dragmacidin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(anti-neurogenic inflammatory compds.)

RN 114582-72-8 HCAPLUS

CN 1H-Indol-4-ol, 6,7-dibromo-3-[(2R,5S)-5-(6-bromo-1H-indol-3-yl)-4-methyl-2-piperazinyl]-, rel-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



L42 ANSWER 28 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:197562 HCAPLUS
DN 128:245177
TI Azo dyes for ink-jet printing
IN Carr, Kathryn; Watson, Anthony Alanzo
PA Zeneca Limited, UK; Carr, Kathryn; Watson, Anthony Alanzo
SO PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9812264	A1	19980326	WO 1997-GB2378	19970905
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9741261	A1	19980414	AU 1997-41261	19970905
	GB 2332440	A1	19990623	GB 1999-2957	19970905
	GB 2332440	B2	20010411		
	US 6277185	B1	20010821	US 1999-269060	19990526
PRAI	GB 1996-19573	A	19960919		
	WO 1997-GB2378	W	19970905		

OS CASREACT 128:245177; MARPAT 128:245177
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The azo dyes have the general formula I (in any suitable form, such as salt, stereoisomer, zwitterion, polymorph, complex, **isotopic** form, combinations thereof), wherein p = 1-7; the naphthyl moiety may be optionally substituted; R1 = H, (un)substituted C1-4 alkyl, NHCO-C1-4-alkyl, C1-4 alkoxy, NHCO-aryl, NHSO2-C1-4-alkyl, NHSO2-aryl, NHCONR3R4; R3, R4 = H, C1-4 alkyl, aryl; R2 = H, C1-4 alkyl, C1-4 alkoxy;

L1, L2 = (un)substituted: -NH2, -NH-C1-4- alkylene-OH, -S-C1-4-alkylene-SO3H, -NH-C1-4-alkylene-N(C1-4-alkyl)2, -N(C1-4-alkylene-OH)2, -NH-C1-4-alkylene-SO3H, -NH-C1-4-alkylene-(CO2H)1-3, -S-C1-4-alkylene-(CO2H)1-3, Q1, Q2; X = NH-C1-4-alkylene, direct link; Y = O, NH; q = 1-7; the naphthyl moiety may be optionally substituted; R5, R6 = H, (un)substituted C1-4 alkyl, NHCO-C1-4- alkyl, C1-4 alkoxy, NHCO-aryl, NHSO2-C1-4-alkyl, NHSO2-aryl, NHCONR7R8; R7, R8 = H, C1-4 alkyl, aryl, and any other suitable labile or non-labile C1-4 alkoxy (optionally substituted with at least one halo), carboxy, sulfo, hydroxy, amino, mercapto, cyano, nitro and halo. II was prepared starting from 2-aminonaphthalene-4,8-disulfonic acid. An ink comprised II 2, water 80, propylene glycol 5, N-methylpyrrolidone 6, di-Me ketone 4, and 2-pyrrolidone 5 parts.

IC ICM C09B043-16
ICS C09D011-00

CC 41-3 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
Section cross-reference(s): 42

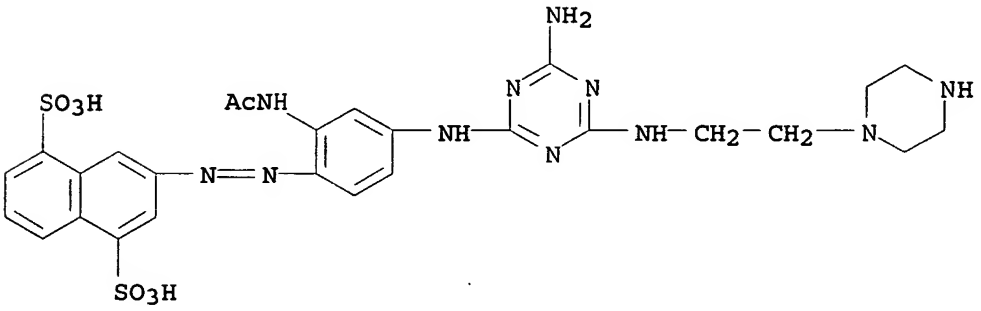
IT 84-94-6P 117-88-4P 53306-14-2P 204712-89-0P 204713-03-1P 204713-09-7P 204713-12-2P 204713-14-4P 204713-16-6P 204713-18-8P 204713-23-5P **204713-26-8P**
RL: IMF (Industrial manufacture); RCT (Reactant); **PREP (Preparation)**; RACT (Reactant or reagent)
(Azo dyes for ink-jet printing)

IT 187674-71-1P 187674-72-2P 204712-93-6P 204713-06-4P 204713-10-0P 204713-13-3P 204713-15-5P 204713-25-7P **204713-27-9P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); **PREP (Preparation)**; USES (Uses)
(Azo dyes for ink-jet printing)

IT **204713-26-8P**
RL: IMF (Industrial manufacture); RCT (Reactant); **PREP (Preparation)**; RACT (Reactant or reagent)
(Azo dyes for ink-jet printing)

RN 204713-26-8 HCAPLUS

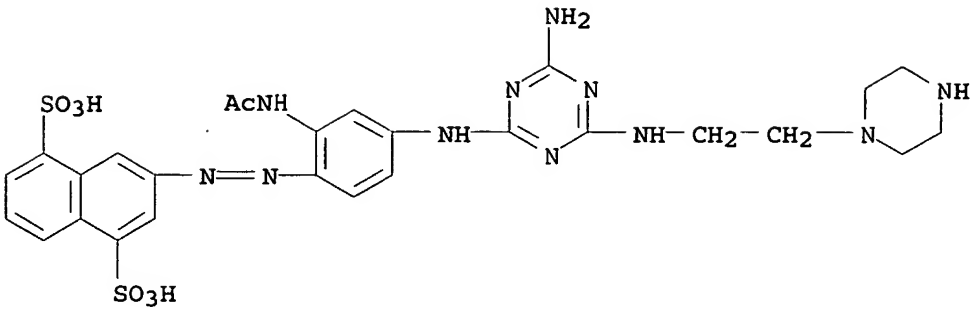
CN 1,5-Naphthalenedisulfonic acid, 3-[[2-(acetylamino)-4-[[4-amino-6-[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazin-2-yl]amino]phenyl]azo]- (9CI) (CA INDEX NAME)



IT **204713-27-9P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); **PREP (Preparation)**; USES (Uses)
(Azo dyes for ink-jet printing)

RN 204713-27-9 HCAPLUS

CN 1,5-Naphthalenedisulfonic acid, 3-[[2-(acetylamino)-4-[[4-amino-6-[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazin-2-yl]amino]phenyl]azo]-, disodium salt (9CI) (CA INDEX NAME)



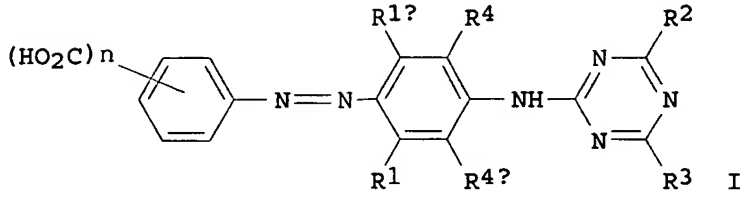
●2 Na

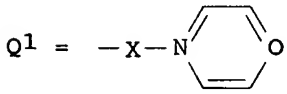
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

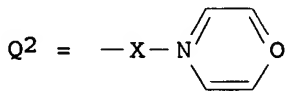
L42 ANSWER 29 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:197561 HCAPLUS
DN 128:245176
TI Azo dyes for ink-jet printing
IN Millard, Christine; Bradbury, Roy; Gregory, Peter
PA Zeneca Limited, UK
SO PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

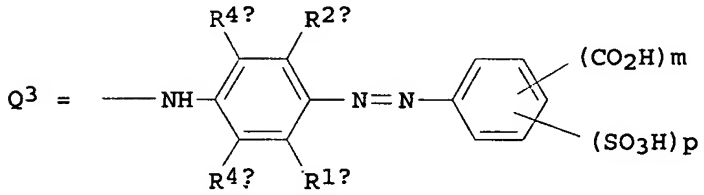
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9812263	A1	19980326	WO 1997-GB2377	19970905
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9741260	A1	19980414	AU 1997-41260	19970715
	GB 2332441	A1	19990623	GB 1999-2959	19970905
	GB 2332441	B2	20010321		
	US 6290763	B1	20010918	US 1999-269061	19990318
PRAI	GB 1996-19570	A	19960919		
	GB 1996-19571	A	19960919		
	GB 1996-19572	A	19960919		
	GB 1996-19574	A	19960919		
	GB 1996-19575	A	19960919		
	GB 1996-19584	A	19960919		
	GB 1996-19585	A	19960919		
	GB 1996-19586	A	19960919		
	GB 1996-19587	A	19960919		
	GB 1996-19588	A	19960919		
	GB 1996-19589	A	19960919		
	GB 1996-19590	A	19960919		

GB 1996-19591 A 19960919
GB 1996-19592 A 19960919
GB 1996-19593 A 19960919
GB 1996-19612 A 19960919
WO 1997-GB2377 W 19970905
OS MARPAT 128:245176
GI









AB The azo dyes have the general formula I (in any suitable form, such as salt; stereoisomer, zwitterion, polymorph, complex, **isotopic** form, combinations thereof), wherein n = 1-5; R1, R1B, R4, R4B = H, (un)substituted C1-8 alkyl, C1-8 alkoxy, -NHCOH, C1-8 alkylcarbonylamino, -NHCONR5R6; R5, R6 = H, C1-8 alkyl, aryl; R2, R3 = H, (un)substituted C1-8 alkoxy, -NH-C1-8-alkylene-OH, -S-C1-8-alkylene-SO3H, -NH-C1-8-alkylene-N(C1-8-alkyl)2, Q1, Q2, Q3; X = -NH-C1-8-alkylene; -NHC6H4SO2NH-C1-8-alkylene, direct link; m, p = 0-5; (m + p) = 1-5; R1A, R2A, R4A, R4C as defined for R1, R2, R4 and R4B resp., and any other suitable labile or non-labile substituent not mentioned above.; the optional substituents may be C1-4-alkyl with or without halo, C1-4-alkoxy with or without halo, carboxy, sulfo, hydroxy, amino, mercapto, cyano, nitro and halo. I (n = 2 for 3,5-dicarboxy; R1 = Me; R1B = R4 = R4B = H; R2 = R3 = SC3H6SO3H) was prepared and converted into ammonium salt. An ink comprised the above ammonium salt 3, water 80, propylene glycol 15, cetylammonium bromide 0.2, and 2-pyrrolidone 5 parts.

IC ICM C09B043-16
ICS C09D011-00

CC 41-3 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
Section cross-reference(s): 42

IT 4889-20-7P 26021-90-9P, Sodium anilinomethanesulfonate 165182-09-2P
204268-42-8P 204268-44-0P 204268-45-1P 204268-47-3P 204268-48-4P
204268-51-9P 204268-52-0P 204268-53-1P 204268-55-3P 204268-57-5P
204268-58-6P 204268-62-2P 204268-64-4P 204268-70-2P 204268-73-5P
204268-76-8P 204268-77-9P **204268-80-4P** 204268-81-5P

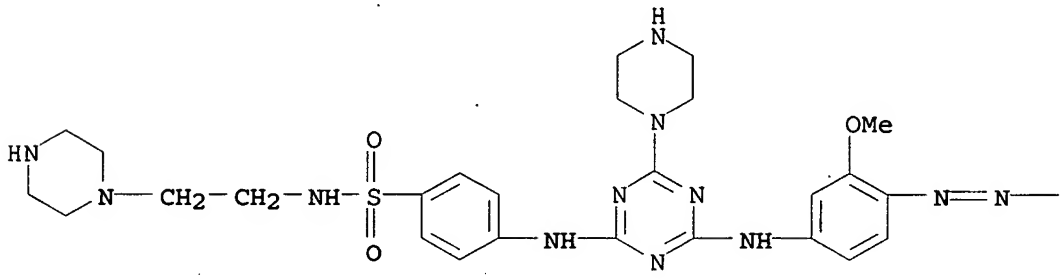
204268-83-7P 204268-84-8P 204268-85-9P 204268-86-0P
204268-87-1P 204268-90-6P 204268-91-7P 204268-92-8P
204268-93-9P 204268-96-2P
RL: IMF (Industrial manufacture); RCT (Reactant); **PREP (Preparation)**; RACT (Reactant or reagent)
(azo dyes for ink-jet printing)

IT 204268-43-9P 204268-46-2P 204268-49-5P 204268-50-8P 204268-54-2P
204268-56-4P 204268-59-7P 204268-60-0P 204268-66-6P 204268-68-8P
204268-74-6P 204268-75-7P 204268-78-0P **204268-79-1P**
204268-82-6P 204268-88-2P 204268-89-3P
204268-94-0P 204268-95-1P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); **PREP (Preparation)**; USES (Uses)
(azo dyes for ink-jet printing)

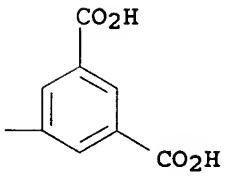
IT **204268-80-4P 204268-83-7P 204268-87-1P**
204268-93-9P 204268-96-2P
RL: IMF (Industrial manufacture); RCT (Reactant); **PREP (Preparation)**; RACT (Reactant or reagent)
(azo dyes for ink-jet printing)

RN 204268-80-4 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[2-methoxy-4-[[4-(1-piperazinyl)-6-[[4-[[[2-(1-piperazinyl)ethyl]amino]sulfonyl]phenyl]amino]-1,3,5-triazin-2-yl]amino]phenyl]azo]- (9CI) (CA INDEX NAME)

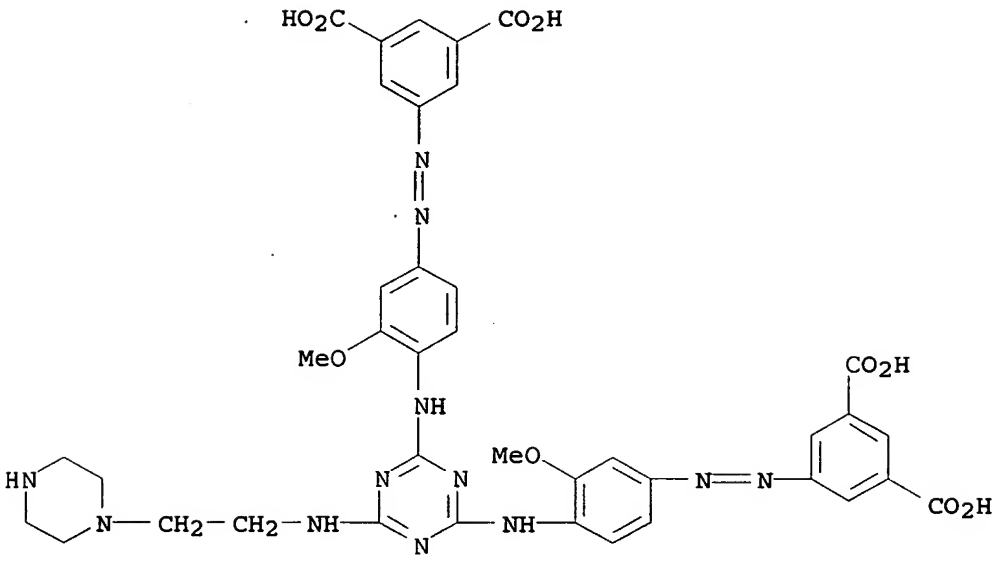
PAGE 1-A



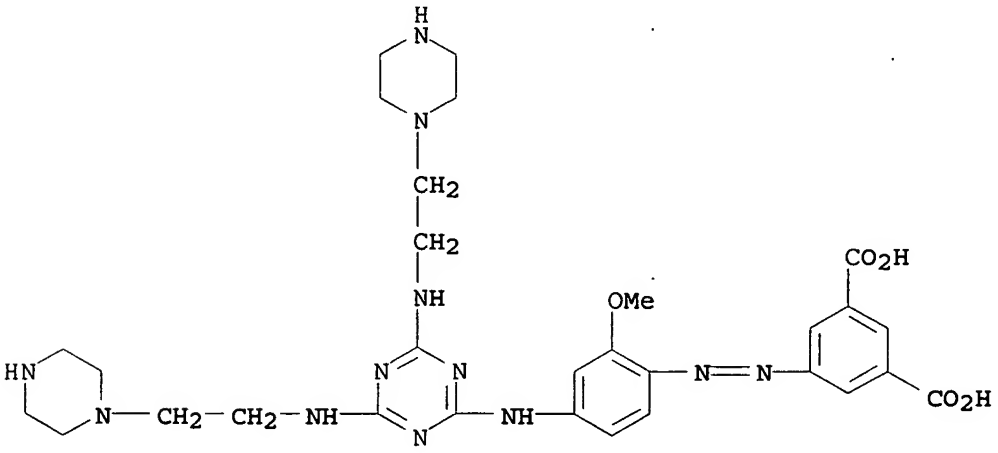
PAGE 1-B



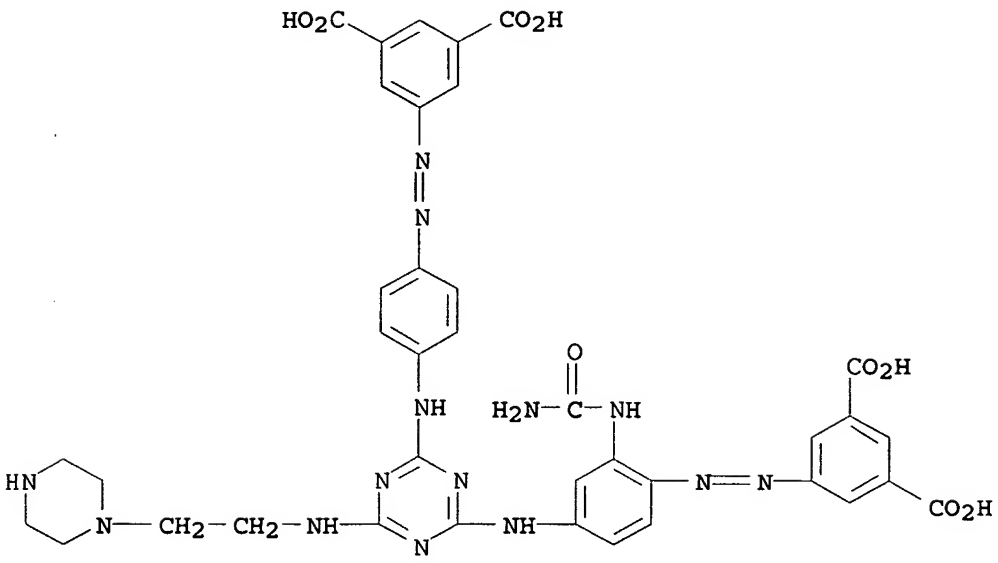
RN 204268-83-7 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5,5'-[[6-[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazine-2,4-diyl]bis[imino(3-methoxy-4,1-phenylene)azo]]bis- (9CI) (CA INDEX NAME)



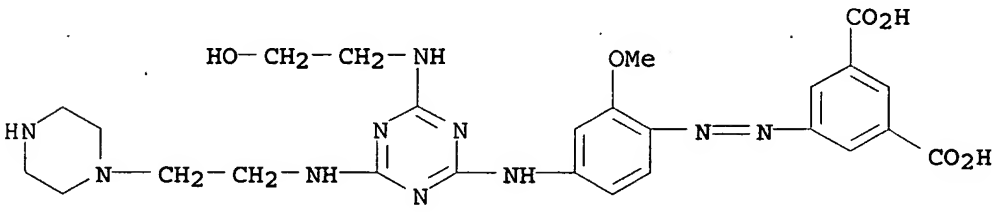
RN 204268-87-1 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[4-[[4,6-bis[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazin-2-yl]amino]-2-methoxyphenyl]azo]- (9CI) (CA INDEX NAME)



RN 204268-93-9 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[2-[(aminocarbonyl)amino]-4-[[4-[[4-[(3,5-dicarboxyphenyl)azo]phenyl]amino]-6-[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazin-2-yl]amino]phenyl]azo]- (9CI) (CA INDEX NAME)

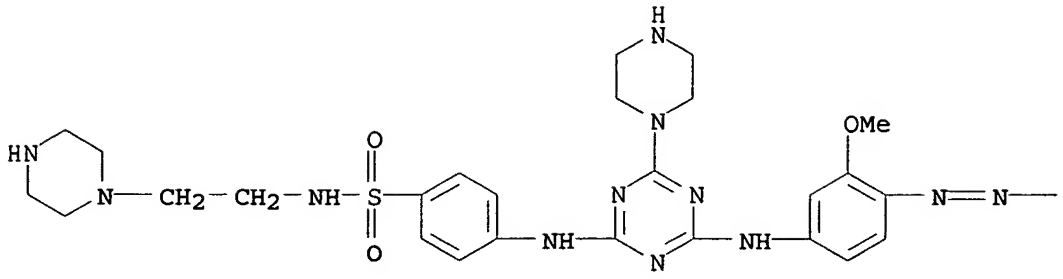


RN 204268-96-2 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[4-[[4-[(2-hydroxyethyl)amino]-6-[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazin-2-yl]amino]-2-methoxyphenyl]azo]-(9CI) (CA INDEX NAME)



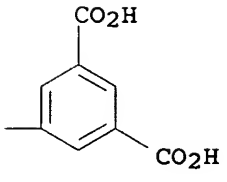
IT **204268-79-1P 204268-82-6P 204268-88-2P**
204268-89-3P 204268-94-0P 204268-95-1P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); **PREP (Preparation)**; USES (Uses)
(azo dyes for ink-jet printing)
RN 204268-79-1 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[2-methoxy-4-[[4-(1-piperazinyl)-6-[[4-[[[2-(1-piperazinyl)ethyl]amino]sulfonyl]phenyl]amino]-1,3,5-triazin-2-yl]amino]phenyl]azo]-, diammonium salt (9CI) (CA INDEX NAME)

PAGE 1-A



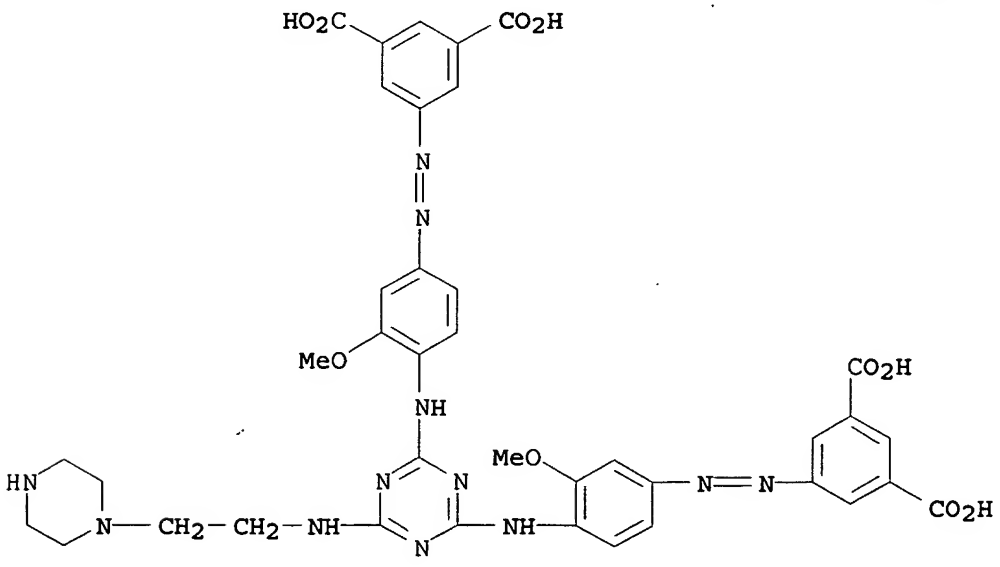
●2 NH_3

PAGE 1-B



RN 204268-82-6 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5,5'-[[6-[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazine-2,4-diyl]bis[imino(3-methoxy-4,1-phenylene)azo]]bis-, tetraammonium salt (9CI) (CA INDEX NAME)

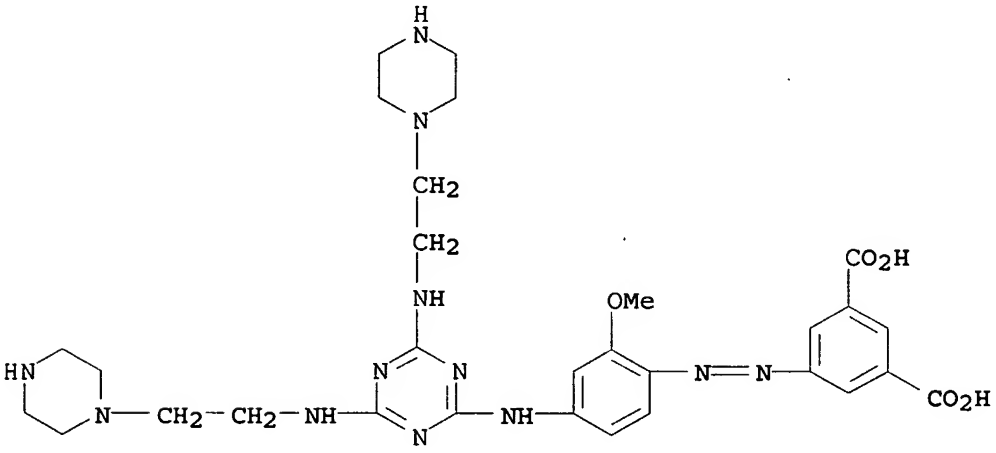
PAGE 1-A



PAGE 2-A

● 4 NH_3

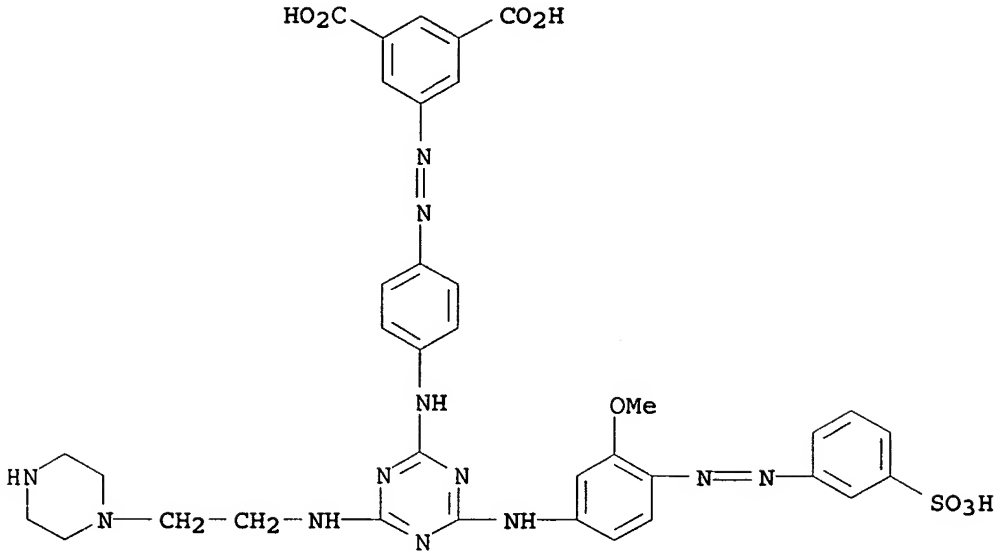
RN 204268-88-2 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[4-[[4,6-bis[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazin-2-yl]amino]-2-methoxyphenyl]azo]-, diammonium salt (9CI) (CA INDEX NAME)



● 2 NH_3

RN 204268-89-3 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[4-[[4-[[3-methoxy-4-[(3-sulfophenyl)azo]phenyl]amino]-6-[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazin-2-yl]amino]phenyl]azo]-, triammonium salt (9CI) (CA INDEX NAME)

PAGE 1-A

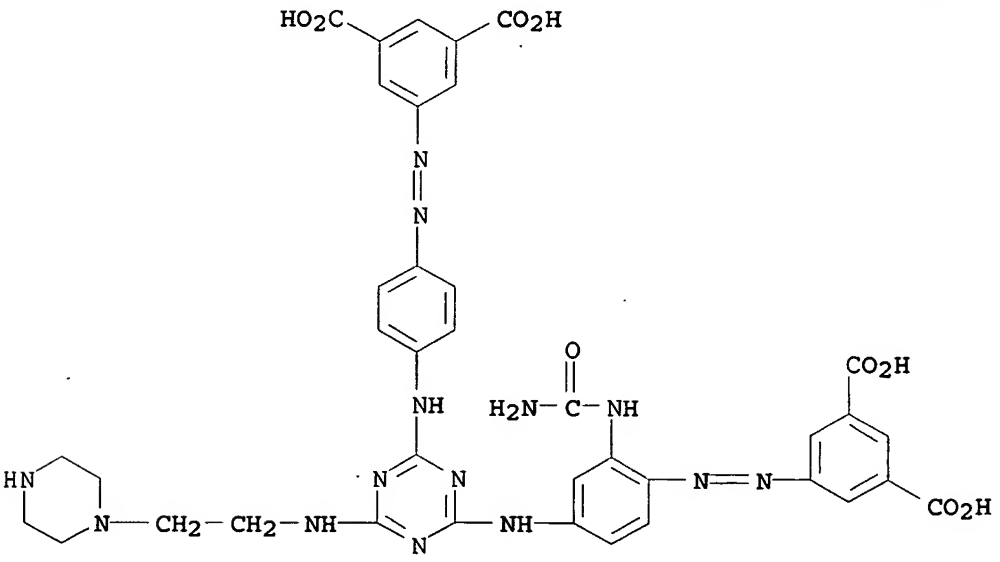


PAGE 2-A

●3 NH_3

RN 204268-94-0 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[2-[(aminocarbonyl)amino]-4-[[4-[[4-[(3,5-dicarboxyphenyl)azo]phenyl]amino]-6-[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazin-2-yl]amino]phenyl]azo]-, tetraammonium salt (9CI) (CA INDEX NAME)

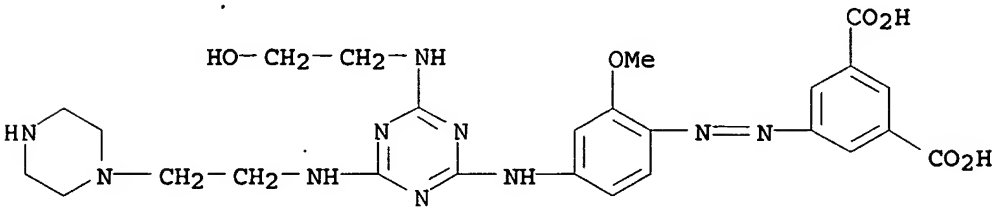
PAGE 1-A



PAGE 2-A

●4 NH_3

RN 204268-95-1 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[4-[[4-[(2-hydroxyethyl)amino]-6-[[2-(1-piperazinyl)ethyl]amino]-1,3,5-triazin-2-yl]amino]-2-methoxyphenyl]azo]-, diammonium salt (9CI) (CA INDEX NAME)



●2 NH_3

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 30 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:689452 HCAPLUS
DN 125:328391
TI Nodulisporic acid derivatives
IN Meinke, Peter T.; Shih, Thomas; Fisher, Michael H.
PA Merck and Co., Inc., USA
SO PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9629073	A1	19960926	WO 1996-US3611	19960315
	W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2215982	AA	19960926	CA 1996-2215982	19960315
	CA 2215982	C	20010612		
	AU 9653134	A1	19961008	AU 1996-53134	19960315
	AU 691424	B2	19980514		
	EP 819000	A1	19980121	EP 1996-909730	19960315
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	JP 10504041	T2	19980414	JP 1996-528529	19960315
	JP 3020279	B2	20000315		
	CN 1184423	A	19980610	CN 1996-193987	19960315
	CN 1082814	B	20020417		
	BR 9607965	A	19980714	BR 1996-7965	19960315

	PL 185563	B1	20030630	PL 1996-322326	19960315
	CZ 294699	B6	20050216	CZ 1997-2935	19960315
	SK 284840	B6	20051201	SK 1997-1259	19960315
	ZA 9602203	A	19960904	ZA 1996-2203	19960319
	TW 534908	B	20030601	TW 1996-85111484	19960919
	NO 9704321	A	19971119	NO 1997-4321	19970919
PRAI	US 1995-406619	A2	19950320		
	US 1996-606312	A2	19960311		
	WO 1996-US3611	W	19960315		

OS MARPAT 125:328391

AB Esters and amides of nodulisporic acid, 29,30-dihydro-20,30-oxanodulisporic acid and 31-hydroxy-20,30-oxa-29,30,31,32-tetrahydronudulic acid (>300 compds.), which are acaricidal, antiparasitic, insecticidal and anthelmintic agents (no data), were prepared Thus, nodulisporic acid was esterified with Me3SiCHN2 to give the Me ester.

IC ICM A61K031-40
ICS A61K031-425; A61K031-445; A61K031-495; C07D405-06; C07D487-16

CC 26-6 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1

IT 183161-04-8P, N-Methylnodulisporamide 183161-06-0P, N-Propylnodulisporamide 183161-07-1P 183161-08-2P 183161-10-6P
183161-11-7P 183161-12-8P 183161-14-0P 183161-15-1P 183161-16-2P
183161-17-3P 183161-18-4P 183161-19-5P, Methyl 1-hydroxynodulisporate
183161-20-8P 183161-21-9P 183161-22-0P 183161-23-1P 183161-24-2P
183161-25-3P 183161-26-4P, 1-Hydroxynodulisporic acid 183161-27-5P
183161-28-6P 183161-29-7P 183284-75-5P 183284-76-6P, Ethyl nodulisporate 183284-77-7P 183284-78-8P 183284-79-9P 183284-80-2P
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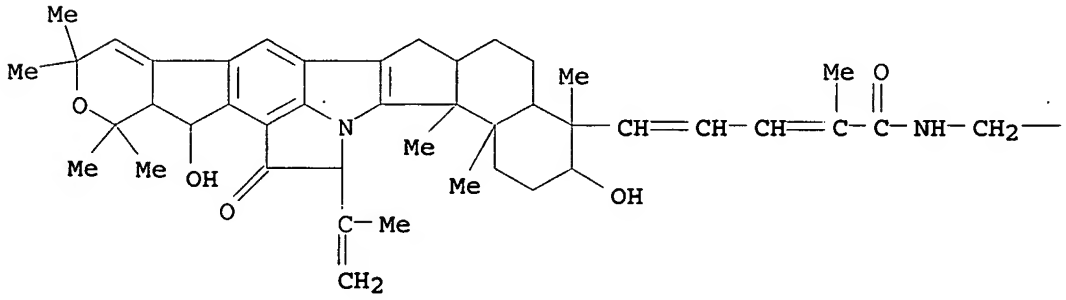
183286-96-6P 183286-97-7P 183286-98-8P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of nodulisporic acid esters and amides as parasiticides)

IT **183285-05-4P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of nodulisporic acid esters and amides as parasiticides)

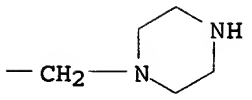
RN 183285-05-4 HCAPLUS

CN 2,4-Pentadienamide, 5-[2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13-dihydroxy-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-14-oxo-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-2-methyl-N-[2-(1-piperazinyl)ethyl]-(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L42 ANSWER 31 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:359973 HCAPLUS
DN 125:103533
TI Multifunctional ligand for use as a diagnostic or therapeutic pharmaceutical
IN Katti, Kattesh V.; Volkert, Wynn A.; Ketring, Alan R.; Singh, Prahlad R.
PA Curators of the University of Missouri, USA
SO U.S., 13 pp., Cont.-in-part of U.S. Ser. No. 50,253, abandoned.
CODEN: USXXAM
DT Patent

LA English
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5516940	A	19960514	US 1994-235355	19940429
	CA 2188569	AA	19951109	CA 1995-2188569	19950327
	WO 9529669	A2	19951109	WO 1995-US3629	19950327
	WO 9529669	A3	20020214		
	W: AU, CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9524598	A1	19951129	AU 1995-24598	19950327
	EP 758887	A1	19970226	EP 1995-918828	19950327
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 09511750	T2	19971125	JP 1995-528219	19950327
PRAI	US 1991-694142	B2	19910501		
	US 1993-50253	B2	19930826		
	US 1994-235355	A	19940429		
	WO 1995-US3629	W	19950327		

OS MARPAT 125:103533
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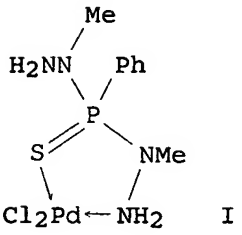


I

AB A compound for use as a diagnostic or therapeutic pharmaceutical comprises either a phosphorus or germanium core and at least two hydrazine groups forming ligand E:PR5(NR2NR3Q)(NR1NR4Q) [R1-R4 = H, selected alkyls, alkylamines, alkoxy groups, aromatic groups; R5 = H, OMe, CH(OH)CH2OH, Me, Ph; E = O or S; Q = H, various (un)substituted CH2Ph or :CHPh], for bonding to a metal extending from the P or Ge core. The ligated metals in the compds. are metallic **isotopes** selected from γ and β emitting **isotopes**, the compds. being stable in aqueous solution, serum, and other body fluids, including 186Re, 188Re, 109Pd, 105Rh, and 99Tc. Also included are paramagnetic metal centers, including Fe and Mn. The compds. may be made by reaction of an appropriate phosphorus halide, E:PCl2X, with a hydrazine, R1R4NNR2R3, for subsequent reaction with a metal compound Thus, reaction of PdCl2(PhCN)2 with PhP(S)(NMeNH2)2 afforded Pd complex I. The compds. are for use as diagnostic and therapeutic pharmaceuticals, or as MRI contrast agents.

IC ICM C07F009-50
ICS C07F009-53; C07D241-04
INCL 564014000
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 1, 8, 29, 63
IT 54529-79-2P 70629-50-4P 80254-53-1P 80265-28-7P 144156-99-0P
144157-00-6P 152967-62-9P 152967-63-0P 152967-64-1P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(phosphorus or germanium hydrazides as ligands in metal complexes

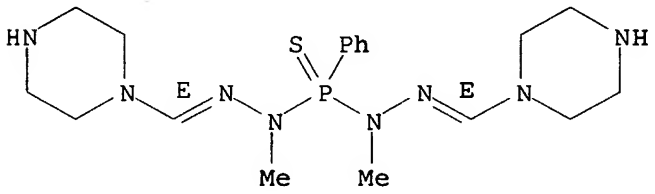
useful as diagnostic or therapeutic pharmaceuticals and MRI contrast agents)

IT 144157-02-8P 144157-04-0P 144157-05-1P 144157-06-2P
144157-07-3P 153090-98-3P 153090-99-4P 153091-00-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(phosphorus or germanium hydrazides as ligands in metal complexes useful as diagnostic or therapeutic pharmaceuticals and MRI contrast agents)

IT **144157-00-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(phosphorus or germanium hydrazides as ligands in metal complexes useful as diagnostic or therapeutic pharmaceuticals and MRI contrast agents)

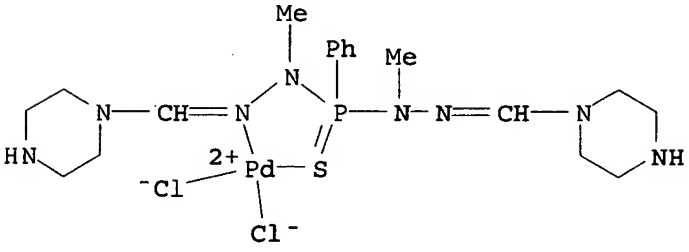
RN 144157-00-6 HCAPLUS
CN Phosphonothioic dihydrazide, 1,1'-dimethyl-P-phenyl-2,2'-bis(1-piperazinylmethylene)-, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **144157-07-3P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(phosphorus or germanium hydrazides as ligands in metal complexes useful as diagnostic or therapeutic pharmaceuticals and MRI contrast agents)

RN 144157-07-3 HCAPLUS
CN Palladium, dichloro[1,1'-dimethyl-P-phenyl-2,2'-bis(1-piperazinylmethylene)phosphonothioic dihydrazide]-, [SP-4-3-(Z,E)]- (9CI) (CA INDEX NAME)

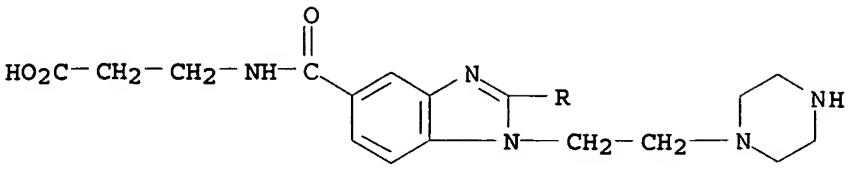


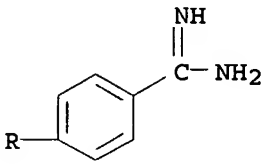
L42 ANSWER 32 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:579485 HCAPLUS
DN 121:179485
TI Preparation of labeled fibrinogen receptor antagonists.
IN Weisenberger, Johannes; Schubert, Hans Dieter; Switek, Karl Heinz; Linz, Guenter; Himmelsbach, Frank

PA Thomae, Dr. Karl, G.m.b.H., Germany
SO Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 567967	A1	19931103	EP 1993-106725	19930426
	EP 567967	B1	19960710		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	DE 4214245	A1	19931104	DE 1992-4214245	19920430
	AT 140225	E	19960715	AT 1993-106725	19930426
	ES 2092170	T3	19961116	ES 1993-106725	19930426
	CA 2094963	AA	19931029	CA 1993-2094963	19930427
	NO 9301528	A	19931029	NO 1993-1528	19930427
	NO 180046	B	19961028		
	NO 180046	C	19970205		
	AU 9337153	A1	19931104	AU 1993-37153	19930427
	AU 670778	B2	19960801		
	JP 06050977	A2	19940225	JP 1993-100789	19930427
	US 5677466	A	19971014	US 1995-477667	19950523
PRAI	DE 1992-4213930	A	19920428		
	DE 1992-4214245	A	19920430		
	US 1993-55176	B1	19930428		

OS MARPAT 121:179485
AB Fibrinogen receptor antagonists having binding affinity ≥ that of 125I-fibrinogen, having in the presence of foreign protein an affinity (Kp) of < 500 nM with respect to the receptor, and having ≥ 1 detectable atom, were prepared Thus, (3S,5S)-5-[(4'-amidino-3-bromo-4-biphenylyl)oxymethyl]-3-[(methoxycarbonyl)methyl]-2-pyrrolidinone hydrochloride (preparation given) in DMF was treated with tritium gas in the presence of Pd/C to give (3S,5S)-5-[(4'-amidino-3-tritio-4-biphenylyl)oxymethyl]-3-[(methoxycarbonyl)methyl]-2-pyrrolidinone hydrochloride of 98.8% radiochem. purity. This was saponified with aqueous NaOH/MeOH to give (3S,5S)-5-[(4'-amidino-3-tritio-4-biphenylyl)oxymethyl]-3-(carboxymethyl)-2-pyrrolidinone (3H-BIBU 52). A curve showing displacement of 3H-BIBU 52 by unlabeled BIBU 52 from human thrombocytes in the presence of plasma is given.
IC ICM C07D401-12
ICS A61K031-395; C07D207-263; C07D207-08; C07D233-72; C07D233-32; C07D249-12; C07D285-10; C07D403-06; C07D211-34; C07C257-18
CC 27-10 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
IT 157446-11-2P 157446-12-3P 157446-13-4P 157446-14-5P 157446-15-6P
157446-16-7P 157446-17-8P 157446-18-9P 157446-19-0P 157446-20-3P
157446-21-4P 157446-22-5P 157446-23-6P 157446-24-7P 157446-25-8P
157446-26-9P 157446-27-0P 157446-28-1P **157446-29-2P**
157446-30-5P 157578-03-5P 157578-04-6P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, as fibrinogen receptor antagonist)
IT **157446-29-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, as fibrinogen receptor antagonist)
RN 157446-29-2 HCAPLUS
CN β-Alanine, N-[[2-[4-(aminoiminomethyl)phenyl]-1-[2-(1-piperazinyl)ethyl]-1H-benzimidazol-5-yl]carbonyl]-, labeled with tritium (9CI) (CA INDEX NAME)





L42 ANSWER 33 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:236178 HCAPLUS
DN 120:236178
TI Use for topsentin compounds and pharmaceutical compositions containing same
IN Mcconnell, Oliver J.; Saucy, Gabriel; Jacobs, Robert
PA Regents of the University of California, USA; Harbor Branch Oceanographic Institute Inc.
SO U.S., 12 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5290777	A	19940301	US 1993-21929	19930224
	CA 2155323	AA	19940901	CA 1994-2155323	19940224
	CA 2155323	C	19940901		
	WO 9419343	A2	19940901	WO 1994-US2031	19940224
	WO 9419343	A3	19941027		
	W: CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 5464835	A	19951107	US 1994-201309	19940224
	EP 686154	A1	19951213	EP 1994-909794	19940224
	EP 686154	B1	19980422		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 09500091	T2	19970107	JP 1994-519282	19940224
	AT 165357	E	19980515	AT 1994-909794	19940224
	ES 2115220	T3	19980616	ES 1994-909794	19940224
	US 5496950	A	19960305	US 1994-330651	19941028
PRAI	US 1993-21929	A	19930224		
	US 1994-201309	A3	19940224		
	WO 1994-US2031	W	19940224		

OS MARPAT 120:236178
AB A novel use for the class of biol. active bis-indole alkaloid compds., which have been named topsentins, nortopsentins, or dragmacidins, pharmaceutical compns. containing them, methods of producing the compds., and methods of using the compds. are disclosed. Specifically, the novel utility pertains to the antiinflammatory properties exhibited by the bis-indole compds. and their analogs. The bis-indole compds. have potent antiinflammatory action in which the mechanism of action appears to be the consequence of inactivation of phospholipase A2. Topsentin and

bromotopsentin were prepared from frozen samples of marine sponge, Spongosorites ruetzleri.

IC ICM A61K031-31
ICS A61K031-495

INCL 514254000

CC 1-7 (Pharmacology)
Section cross-reference(s): 7, 12, 28

IT 112515-42-1 116725-88-3, **Isotopsentin** 116725-89-4, Hydroxytopsentin 116725-90-7, Neotopsentin 116725-91-8, Neoisotopsentin 116747-41-2, Neohydroxytopsentin 154269-22-4 154269-23-5
RL: BIOL (Biological study)
(as antiinflammatory agent)

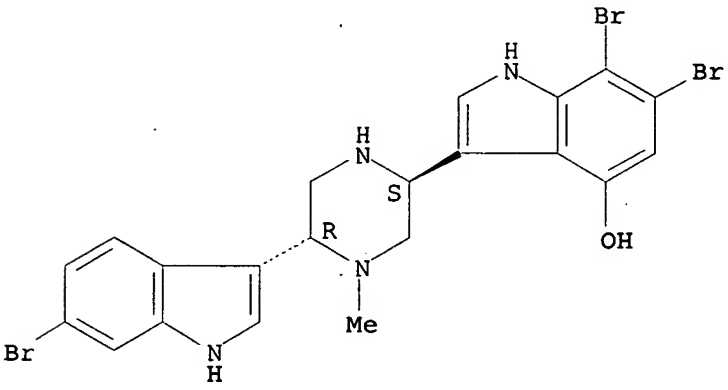
IT 112515-43-2P 112515-44-3P, Bromotopsentin **114582-72-8P**, Dragmacidin 134029-43-9P, Nortopsentin A 134029-44-0P, Nortopsentin B 134029-45-1P, Nortopsentin C
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); **PREP (Preparation)**
(purification and antiinflammatory activity of)

IT **114582-72-8P**, Dragmacidin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); **PREP (Preparation)**
(purification and antiinflammatory activity of)

RN 114582-72-8 HCAPLUS

CN 1H-Indol-4-ol, 6,7-dibromo-3-[(2R,5S)-5-(6-bromo-1H-indol-3-yl)-4-methyl-2-piperazinyl]-, rel-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



L42 ANSWER 34 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1992:465659 HCAPLUS

DN 117:65659

TI Iodine-125- and fluorine-18-labeled aryl-1,4-dialkylpiperazines: potential radiopharmaceuticals for in vivo study of the dopamine uptake system

AU Van Dort, Marcian E.; Kilbourn, Michael R.; Chakraborty, Pulak K.; Richfield, Eric K.; Gildersleeve, David L.; Wieland, Donald M.

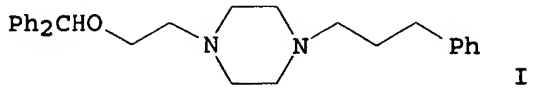
CS Med. Sch., Univ. Michigan, Ann Arbor, MI, 48109, USA

SO Applied Radiation and Isotopes (1992), 43(5), 671-80
CODEN: ARISEF; ISSN: 0883-2889

DT Journal

LA English

GI



I

AB A series of fluorine-18 and iodine-125-labeled aryl-1,4-dialkylpiperazine analogs, derivs. of GBR 12935 (I) were prepared as radiotracers for positron emission tomog. or single photon emission computerized tomog. imaging of the brain based on their affinity for the presynaptic dopamine reuptake system. High specific activity fluorine-18 tracers were prepared by nucleophilic aromatic substitution reactions; iodine-125 tracers were prepared by **isotopic** exchange reactions. In vitro competitive binding studies demonstrated that iodine substitution is tolerated in the 4-position of the Ph ring of the phenalkylpiperazine group. In vivo regional brain biodistribution studies in mice indicated no selectivity of the radioiodinated ligands for the dopamine reuptake site, with striatum/cerebellum concentration ratios of 1. Similar neg. results with the new fluorine-18 derivs. demonstrated that in vivo selectivity for the dopamine reuptake site appears to be critically dependent on the carbon chain length between the piperazine ring and the solitary aromatic ring. Development of new radiopharmaceuticals based on the GBR 12935 structure cannot be based solely on considerations of in vitro binding affinities.

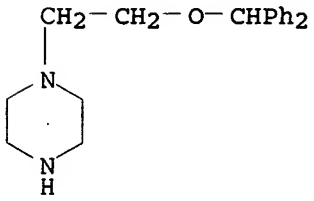
CC 8-9 (Radiation Biochemistry)
Section cross-reference(s): 28

IT **60703-69-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and substitution reaction of, with (iodophenyl)propyl tosylates)

IT **60703-69-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and substitution reaction of, with (iodophenyl)propyl tosylates)

RN 60703-69-7 HCAPLUS

CN Piperazine, 1-[2-(diphenylmethoxy)ethyl]- (6CI, 9CI) (CA INDEX NAME)



L42 ANSWER 35 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1992:193448 HCAPLUS

DN 116:193448

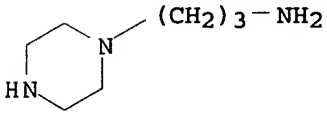
TI Nucleophilic cleavage and formation of saturated heterocycles. XII. Reactivity of small heterocycles in aminolysis and hydrolysis

AU Bobylev, V. A.; Veselkov, N. Yu.; Dalin, A. R.; Sharikov, F. Yu.

CS NPO Gos. Inst. Prikl. Khim., Leningrad, USSR

SO Zhurnal Obshchei Khimii (1991), 61(8), 1841-56
CODEN: ZOKHA4; ISSN: 0044-460X

DT Journal
LA Russian
AB Cleavage reactions of azetidine and oxetane had more product-like transition states than cleavage reactions of aziridine and oxirane. The O heterocycles reacted with general acid catalysis, the N heterocycles with specific acid catalysis. The reactivity of amines in the opening of azetidine depended linearly on pKa, primary and secondary amines forming sep. reaction series.
CC 22-5 (Physical Organic Chemistry)
IT **Isotope** effect
(in hydrolysis of oxetane, by deuterium)
IT 7782-39-0, Deuterium, properties
RL: PRP (Properties)
(**isotope** effect of, in hydrolysis of oxetane)
IT 104-78-9P 123-00-2P, 4-Morpholinepropanamine 3529-08-6P, 1-Piperidinepropanamine 4461-39-6P 13531-52-7P 18169-30-7P 23764-31-0P **34885-02-4P**, 1-Piperazinepropanamine 52198-64-8P 103502-67-6P
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and mass spectrum of)
IT **34885-02-4P**, 1-Piperazinepropanamine
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and mass spectrum of)
RN 34885-02-4 HCAPLUS
CN 1-Piperazinepropanamine (9CI) (CA INDEX NAME)



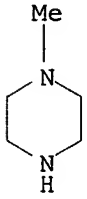
L42 ANSWER 36 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1989:135210 HCAPLUS
DN 110:135210
TI Synthesis of [3H]clozapine
AU De Paulis, Tomas; Davis, Daniel A.; Smith, Howard E.; Malarek, David H.; Liebman, Arnold A.
CS Dep. Chem., Vanderbilt Univ., Nashville, TN, 37235, USA
SO Journal of Labelled Compounds and Radiopharmaceuticals (1988), 25(9), 1027-33
CODEN: JLCRD4; ISSN: 0362-4803
DT Journal
LA English
OS CASREACT 110:135210
AB [3H]clozapine was prepared with a specific activity of 9.9 Ci/mmol by reaction of 8-chloro-11-(methylthio)-5H-dibenzo[b,e][1,4]diazepine with an excess of [3H]N-methylpiperazine. The latter was prepared from N-methylpyrazinium bromide in ethanolic HCl by reduction at room temperature with tritium over 5% Rh on Al2O3.
CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **119550-27-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and condensation reaction of, with dibenzodiazepine derivative,

labeled clozapine from)

IT **119550-27-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and condensation reaction of, with dibenzodiazepine derivative, labeled clozapine from)

RN 119550-27-5 HCAPLUS

CN Piperazine, 1-methyl-, labeled with tritium (9CI) (CA INDEX NAME)



L42 ANSWER 37 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1982:192816 HCAPLUS

DN 96:192816

TI Analysis of plasma trifluoperazine by gas chromatography and selected ion monitoring

AU Whelpton, Robin; Curry, Stephen H.; Watkins, Geraldine M.

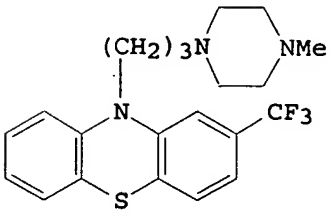
CS Med. Coll., London Hosp., London, E1 2AD, UK

SO Journal of Chromatography (1982), 228, 321-6
CODEN: JOCRAM; ISSN: 0021-9673

DT Journal

LA English

GI



I

AB Following extraction from rat and human plasma, and 2 back-extns., trifluoperazine (I) [117-89-5] was determined by gas chromatog. on 3% OV-225 on Chromosorb W HP and mass spectrometry, using selective ion monitoring of an internal standard labeled with a stable **isotope.** The internal standard used was trifluoperazine-d3 dimaleate [81498-91-1], the synthesis and deuteration of which are described. Measurements were made at m/e 407 for I and m/e 410 for the standard The calibration plot was linear over the range 0.5-200 mg I/mL. The limit of detection was 160-400 pg/mL, depending on the sample volume injected. Preliminary data suggested that this method was suitable for assaying plasma for sufficient time to derive pharmacokinetic data after a single oral I dose.

CC 1-1 (Pharmacology)

IT **3935-47-5P**

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and deuteromethylation of)

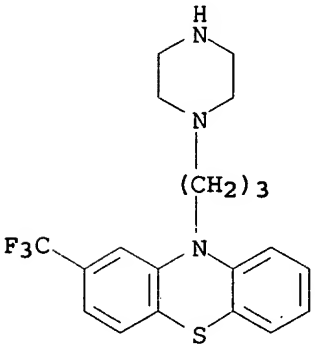
IT **3935-47-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and deuteromethylation of)

RN 3935-47-5 HCAPLUS

CN 10H-Phenothiazine, 10-[3-(1-piperazinyl)propyl]-2-(trifluoromethyl)-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

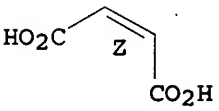
CRN 2804-16-2
CMF C20 H22 F3 N3 S



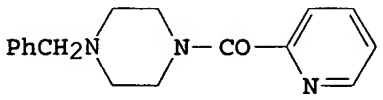
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



L42 ANSWER 38 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1981:462131 HCAPLUS
DN 95:62131
TI Synthesis of carbon-14 and tritium specifically labeled 1-benzyl-4-picolinoylpiperazine
AU Zolyomi, G.; Budai, Z.
CS Inst. Drug Res., Budapest, H-1325, Hung.
SO Journal of Labelled Compounds and Radiopharmaceuticals (1981), 18(3), 427-32
CODEN: JLCRD4; ISSN: 0362-4803
DT Journal
LA English
OS CASREACT 95:62131
GI



I

AB Regiospecifically labeled 1-benzyl-4-picolinoylpiperazine I was prepared for use in metabolism studies by the condensation reaction of benzylpiperazine with picolinic acid. By the use of labeled reactants 14C was introduced both in the benzyl and picolinoyl groups and T in the benzyl group.

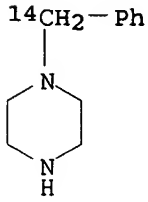
CC 28-18 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 27

IT **78387-77-6P** 78387-78-7P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and condensation reaction of, with picolinic acid)

IT **78387-77-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and condensation reaction of, with picolinic acid)

RN 78387-77-6 HCAPLUS

CN Piperazine, 1-(phenylmethyl-14C)- (9CI) (CA INDEX NAME)



L42 ANSWER 39 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1974:37072 HCAPLUS

DN 80:37072

TI Synthesis of 4,4'-difluorobenzhydryl-α-14C-1-piperazine

AU Donnert, D.; Schweer, K. H.

CS Inst. Radiochem., Ges. Kernforsch., Karlsruhe, Fed. Rep. Ger.

SO Journal of Labelled Compounds (1973), 9(3), 405-12
CODEN: JLCAAI; ISSN: 0022-2135

DT Journal

LA German

GI For diagram(s), see printed CA Issue.

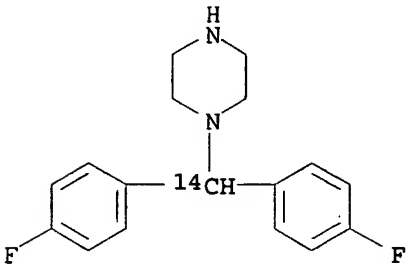
AB 4,4'-Difluorobenzhydryl-α-14C-1-piperazine (I) was prepared from Ba14CO3 and p-FC6H4Br. The identity of the labeled compound was established by comparison with the unlabeled one, synthesized by the same method. The latter was identified with the aid of elementary analysis, mass- and ir spectroscopy.

CC 28-18 (Heterocyclic Compounds (More Than One Hetero Atom))

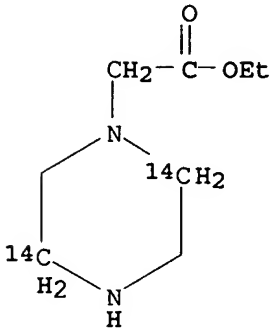
IT 1523-98-4P 51323-52-5P 51323-53-6P **51323-54-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

IT **51323-54-7P**

RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 51323-54-7 HCAPLUS
CN Piperazine, 1-[bis(4-fluorophenyl)methyl-14C]- (9CI) (CA INDEX NAME)



L42 ANSWER 40 OF 40 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1972:475189 HCAPLUS
DN 77:75189
TI Synthesis of ethyl 4-(3,4,5-trimethoxycinamoyl)-[2,5-14C]piperazinyl acetate and ethyl 4-(3,4,5-trimethoxy[β-14C]cinnamoyl)piperazinyl acetate
AU Hardy, G.; Sword, I. P.; Hathway, D. E.
CS Dep. Metab. Stud., Huntingdon Res. Cent., Huntingdon, UK
SO Journal of Labelled Compounds (1972), 8(2), 221-30
CODEN: JLCAAI; ISSN: 0022-2135
DT Journal
LA English
AB Et 4-(3,4,5-trimethoxycinnamoyl)piperazinyl-2,5-14C acetate was prepared from piperazine-2,5-14C, and Et piperazinyl-2,5-14C acetate, and Et 4-(3,4,5-trimethoxycinnamoyl-β-14C)-piperazinyl acetate was prepared from 3,4,5-trimethoxybromobenzene and 3,4,5-trimethoxybenzaldehyde-α-14C.
CC 28-18 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 2539-27-7P 2675-79-8P 37024-12-7P **37024-13-8P** 37024-14-9P 37024-16-1P 38420-54-1P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
IT **37024-13-8P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 37024-13-8 HCAPLUS
CN 1-Piperazine-2,5-14C2-acetic acid, ethyl ester (9CI) (CA INDEX NAME)



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